

# CP Violation in the General Two-Higgs-Doublet Model: a Geometric View

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We discuss the CP properties of the potential in the general Two-Higgs-Doublet Model (THDM). This is done in a concise way using real gauge invariant functions built from the scalar products of the doublet fields. The space of these invariant functions, parametrising the gauge orbits of the Higgs fields, is isomorphic to the forward light cone and its interior. CP transformations are shown to correspond to reflections in the space of the gauge invariant functions. We consider CP transformations where no mixing of the Higgs doublets is taken into account as well as the general case where the Higgs basis is not fixed. We present basis independent conditions for explicit CP violation which may be checked easily for any THDM potential. Conditions for spontaneous CP violation, that is CP violation through the vacuum expectation values of the Higgs fields, are also derived in a basis independent way.

## 1. INTRODUCTION

In the Standard Model (SM) and in many extensions of it like the Minimal Supersymmetric Standard Model (MSSM) [1, 2] the electroweak symmetry breaking is accomplished via the Higgs mechanism. In the SM, where one Higgs doublet is introduced, the Higgs potential is automatically invariant under CP transformations. Thus, CP violation in the SM only arises via Yukawa interactions of the Higgs field with the fermions, that is, through the Kobayashi–Maskawa mechanism [3].

Here we investigate models having the standard weak isospin times hypercharge ( $SU(2)_L \times U(1)_Y$ ) gauge group as invariance group and a Higgs sector with two doublets. That is, we consider the general Two-Higgs-Doublet Model (THDM). In contrast to the SM, in the THDM the Higgs potential itself is in general not invariant under CP transformations [3].

The CP properties of the Higgs potential are studied in the framework of gauge invariant functions, built from all possible  $SU(2)_L \times U(1)_Y$  invariant scalar products of Higgs doublets [4]. In this approach all invariant scalar products are replaced by real gauge invariant functions which can be combined to a four-vector. In terms of these real gauge invariant functions a mixing of the Higgs doublets corresponds to rotations of the *space-like* components of this four-vector and, as we shall show, CP transformations correspond to reflections of the *space-like* components. Thus, constraints for CP invariance can be derived concisely in this geometric picture. We also give unambiguous criteria for the occurrence of *spontaneous* CP violation, where CP violation arises from the vacuum expectation values of the Higgs doublets, although the Higgs potential itself is CP invariant.

There is much interest in the investigation of an exten-

sion of the Higgs sector for several reasons: supersymmetric extensions require one to have at least two Higgs doublets in order to give masses to up- and down-type fermions and to keep the theory anomaly free. Generally, the *naturalness* problem arising in the SM is crucially depending on the Higgs sector. In [5] this has been used as a motivation to focus on the THDM. For a recent proposal of THDMs having a *custodial symmetry* see [6]. Another reason originating from cosmology is that CP violation is one of the three Sakharov criteria which have to be fulfilled in order to explain the observed baryon–antibaryon asymmetry in our Universe through the particle dynamics [7, 8]. In the SM, given the strength of the observed CP violation and the experimental lower bound on the Higgs mass, one cannot explain the baryon excess over anti-baryons observed in our Universe. For a review see for instance [9]. A possible way out of this dilemma is to consider models with an extended Higgs sector.

There exists already an extensive literature on CP violation in multi-Higgs and, in particular, two-Higgs-doublet models. A general discussion of CP transformations in gauge theories was given in [10]. In [11, 12] basis independent conditions for spontaneous CP violation are given for the general THDM. References [13, 14] provide an extensive analysis of the general THDM in terms of invariants with respect to  $U(2)$  Higgs basis changes. In [13] a proof is given that the conditions of [11] for spontaneous CP violation are sufficient and necessary. Reference [14] determines the necessary and sufficient conditions for explicit CP violation in a basis independent way via the systematic check of potentially complex invariants. A rather detailed account of CP violation in N-Higgs-doublet models in general and THDMs in particular was given in [15] using gauge invariant functions. In [17] the Higgs mass squared matrix is considered and CP-conservation conditions are determined from the possible mixing of CP-even and CP-odd entries in this matrix. Reference [16] is devoted to spontaneous symmetry breaking in THDMs, focusing critically on the issue if and when the usual parameter  $\tan\beta$  can be considered to be a truly physical parameter. A measure for CP violating effects is dis-

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cussed in [18] for a given Higgs basis and vacuum. Let us also mention the investigation of the minima structure of THDMs in context with CP violation; see [19] and references therein. In [20] the THDM was studied from a group theoretic point of view. In [21, 22] the Minkowski space structure of the  $\tilde{\mathbf{K}}$ -space (in our notation) was emphasised. Lorentz transformations were used to diagonalise the term of the potential  $V$  (24) quadratic in  $\tilde{\mathbf{K}}$ . In our present paper we have not used Lorentz transformations in  $\tilde{\mathbf{K}}$ -space for several reasons. Lorentz transformations do in general not respect the form of the kinetic term in the Higgs Lagrangian. In [23] we are interested in the complete theory. Thus we only consider Higgs-basis transformations which keep the kinetic term invariant. There are potentials which are stable in the weak sense (see section 4 of [4]) and thus completely acceptable from a physical point of view. We find examples of such potentials where the term quadratic in  $\tilde{\mathbf{K}}$  cannot be diagonalised by a Lorentz transformation. In our work we do not exclude these cases from the discussion. Also we find it generally advantageous to give criteria for properties of a THDM in a way directly applicable for any given model without assuming a particular choice for the Higgs-flavour basis.

In our present paper we take up again the question of CP violation in THDMs. We derive some new results and rederive already known results in a way as we need it for the companion paper [23]. Indeed, the present paper and [23] should be considered as belonging together and forming one unit. Our present paper is organised as follows. In section 2 we briefly recall the definitions of the gauge invariant functions which provide our framework to investigate CP properties. Then, in section 3, we classify the possible types of CP transformations and present constraints for CP invariance of the potential in this framework. This is followed in section 4 by a discussion of spontaneous CP violation. The general results are illustrated in section 5, where we discuss two specific models in the more conventional parametrisation of [24]. Section 6 contains our conclusions. In the respective sections we also compare our findings to those in the literature mentioned above. The appendices contain the proofs of two theorems and details for general models with different types of CP symmetries.

## 2. GAUGE INVARIANT FUNCTIONS IN THE GENERAL TWO-HIGGS-DOUBLET MODEL

We shall use the gauge invariant functions as introduced in [4]. Here we recall the formalism briefly in order to make this work self-contained.

We denote the two complex Higgs-doublet fields by

$$\varphi_i(x) = \begin{pmatrix} \varphi_i^+(x) \\ \varphi_i^0(x) \end{pmatrix} \quad (1)$$

with  $i = 1, 2$ . Hence we have eight real scalar degrees of freedom. The most general  $SU(2)_L \times U(1)_Y$  invariant

Lagrangian for the THDM can be written as

$$\mathcal{L}_{\text{THDM}} = \mathcal{L}_\varphi + \mathcal{L}_{\text{Yuk}} + \mathcal{L}', \quad (2)$$

where the Higgs-boson Lagrangian is given by

$$\mathcal{L}_\varphi = \sum_{i=1,2} (\mathcal{D}_\mu \varphi_i)^\dagger (\mathcal{D}^\mu \varphi_i) - V(\varphi_1, \varphi_2). \quad (3)$$

This term replaces the kinetic terms of the Higgs boson and the Higgs potential in the SM Lagrangian. The covariant derivative is

$$\mathcal{D}_\mu = \partial_\mu + igW_\mu^a \mathbf{T}_a + ig' B_\mu \mathbf{Y}, \quad (4)$$

where  $\mathbf{T}_a$  and  $\mathbf{Y}$  are the generating operators of weak-isospin and weak-hypercharge transformations. For the Higgs doublets we have  $\mathbf{T}_a = \tau_a/2$ , where  $\tau_a$  ( $a = 1, 2, 3$ ) are the Pauli matrices. We assume both doublets to have weak hypercharge  $y = +1/2$ . By  $\mathcal{L}_{\text{Yuk}}$  we denote the Yukawa-interaction terms of the Higgs fields with the fermions. Finally,  $\mathcal{L}'$  contains the terms of the Lagrangian without Higgs fields. We do not specify  $\mathcal{L}_{\text{Yuk}}$  and  $\mathcal{L}'$  here since they are not relevant for our analysis.

We remark that in the MSSM the two Higgs doublets  $H_1$  and  $H_2$  carry hypercharges  $y = -1/2$  and  $y = +1/2$ , respectively, whereas here we use the conventional definition of the THDM with both doublets carrying  $y = +1/2$ . However, our analysis can be translated to the other case, see for example (3.1) in [25], by setting

$$\begin{aligned} \varphi_1^\alpha &= -\epsilon_{\alpha\beta} (H_1^\beta)^*, \\ \varphi_2^\alpha &= H_2^\alpha, \end{aligned} \quad (5)$$

where  $\epsilon$  is given by

$$\epsilon = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (6)$$

The most general gauge invariant and renormalisable potential  $V(\varphi_1, \varphi_2)$  for the two Higgs doublets  $\varphi_1$  and  $\varphi_2$  is a hermitian linear combination of the following terms:

$$\varphi_i^\dagger \varphi_j, \quad (\varphi_i^\dagger \varphi_j)(\varphi_k^\dagger \varphi_l), \quad (7)$$

where  $i, j, k, l \in \{1, 2\}$ . It is convenient to discuss the properties of the potential in terms of gauge invariant expressions. For this purpose we arrange the fields  $\varphi_i$  (1) in a  $2 \times 2$  matrix (see (A.2) of [4])

$$\phi(x) = \begin{pmatrix} \varphi_1^+(x) & \varphi_1^0(x) \\ \varphi_2^+(x) & \varphi_2^0(x) \end{pmatrix}. \quad (8)$$

Similarly, we arrange the  $SU(2)_L \times U(1)_Y$  invariant scalar products into the hermitian  $2 \times 2$  matrix

$$\underline{K}(x) := \begin{pmatrix} \varphi_1^\dagger \varphi_1 & \varphi_1^\dagger \varphi_2 \\ \varphi_2^\dagger \varphi_1 & \varphi_2^\dagger \varphi_2 \end{pmatrix} = \phi(x) \phi^\dagger(x) \quad (9)$$

and consider its decomposition

$$\underline{K}_{ij}(x) = \frac{1}{2} (K_0(x) \delta_{ij} + K_a(x) \sigma_{ij}^a), \quad (10)$$

using the completeness of the Pauli matrices  $\sigma^a$  ( $a = 1, 2, 3$ ) together with the unit matrix. Here and in the following summation over repeated indices is understood. Explicitly, (9) and (10) yield

$$\begin{aligned}\varphi_1^\dagger \varphi_1 &= (K_0 + K_3)/2, & \varphi_1^\dagger \varphi_2 &= (K_1 + iK_2)/2, \\ \varphi_2^\dagger \varphi_2 &= (K_0 - K_3)/2, & \varphi_2^\dagger \varphi_1 &= (K_1 - iK_2)/2.\end{aligned}\quad (11)$$

Thus the four real coefficients defined by the decomposition (10) are given by

$$\begin{aligned}K_0 &= \varphi_1^\dagger \varphi_1 + \varphi_2^\dagger \varphi_2, & K_1 &= 2 \operatorname{Re} \varphi_1^\dagger \varphi_2, \\ K_3 &= \varphi_1^\dagger \varphi_1 - \varphi_2^\dagger \varphi_2, & K_2 &= 2 \operatorname{Im} \varphi_1^\dagger \varphi_2.\end{aligned}\quad (12)$$

Using the three-vector notation

$$\mathbf{K}(x) := \begin{pmatrix} K_1(x) \\ K_2(x) \\ K_3(x) \end{pmatrix}, \quad (13)$$

the most general potential can be written as follows:

$$V = \xi_0 K_0 + \boldsymbol{\xi}^T \mathbf{K} + \eta_{00} K_0^2 + 2K_0 \boldsymbol{\eta}^T \mathbf{K} + \mathbf{K}^T E \mathbf{K}, \quad (14)$$

with

$$\boldsymbol{\xi} := \begin{pmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \end{pmatrix}, \quad \boldsymbol{\eta} := \begin{pmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{pmatrix}, \quad E := \begin{pmatrix} \eta_{11} & \eta_{12} & \eta_{13} \\ \eta_{21} & \eta_{22} & \eta_{23} \\ \eta_{31} & \eta_{32} & \eta_{33} \end{pmatrix}. \quad (15)$$

Here the 14 independent potential parameters  $\xi_0, \xi_a, \eta_{00}, \eta_a$  and  $\eta_{ab} = \eta_{ba}$  are real.

Now we consider a change of basis of the Higgs fields,  $\varphi_i \rightarrow \varphi'_i$ , where

$$\begin{pmatrix} \varphi'_1 \\ \varphi'_2 \end{pmatrix} = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}. \quad (16)$$

Here

$$U = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}, \quad U^\dagger U = \mathbb{1}_2, \quad (17)$$

is a  $2 \times 2$  unitary matrix. With (16) the gauge invariant functions (12) transform as

$$K'_0 = K_0, \quad K'_a = R_{ab}(U) K_b, \quad (18)$$

where  $R_{ab}(U)$  is defined by

$$U^\dagger \sigma^a U = R_{ab}(U) \sigma^b. \quad (19)$$

The matrix  $R(U)$  has the properties

$$R^*(U) = R(U), \quad R^T(U) R(U) = \mathbb{1}_3, \quad \det R(U) = 1, \quad (20)$$

where  $\mathbb{1}_3$  denotes the  $3 \times 3$  unit matrix. The transformations fulfill  $R(U) \in SO(3)$ , that is, they are proper rotations in  $\mathbf{K}$ -space.

The Higgs potential (14) remains unchanged under the replacements (18) if we perform an appropriate transformation of the parameters of  $V$ :

$$\begin{aligned}\xi'_0 &= \xi_0, & \boldsymbol{\xi}' &= R(U) \boldsymbol{\xi}, \\ \eta'_{00} &= \eta_{00}, & \boldsymbol{\eta}' &= R(U) \boldsymbol{\eta}, \\ E' &= R(U) E R^T(U).\end{aligned}\quad (21)$$

Moreover, for every matrix  $R$  with the properties (20), there is a unitary transformation (16). We can therefore diagonalise  $E$ , thereby reducing the number of parameters of  $V$  by three. The Higgs potential is then determined by only 11 real parameters.

The matrix  $\underline{K}(x)$  is positive semi-definite, which follows immediately from its definition (9). With  $K_0 = \operatorname{tr} \underline{K}$  and  $K_0^2 - \mathbf{K}^2 = 4 \det \underline{K}$  this implies

$$K_0(x) \geq 0, \quad K_0(x)^2 - \mathbf{K}(x)^2 \geq 0. \quad (22)$$

On the other hand, for any given  $K_0(x), \mathbf{K}(x)$  fulfilling (22), it is possible to find fields  $\varphi_i$  obeying (12). Furthermore, all fields obeying (12) for a given  $K_0(x), \mathbf{K}(x)$  form one gauge orbit; see appendix A of [4].

Thus, the functions  $K_0(x), K_a(x)$  parametrise the gauge orbits and not a unique Higgs-field configuration. Specifying the domain of the functions  $K_0(x), K_a(x)$  corresponding to the gauge orbits allows to discuss the potential directly in the form (14) with all gauge degrees of freedom eliminated. We note that the gauge orbits of the Higgs fields of the THDM are parametrised by Minkowski type four-vectors

$$\tilde{\mathbf{K}}(x) = \begin{pmatrix} K_0(x) \\ \mathbf{K}(x) \end{pmatrix} \quad (23)$$

which have to lie on or inside the forward light cone. This allows us to write the most general potential (14) in the concise form (see (87) and (88) of [4])

$$V = \tilde{\mathbf{K}}^T \tilde{\boldsymbol{\xi}} + \tilde{\mathbf{K}}^T \tilde{E} \tilde{\mathbf{K}}, \quad (24)$$

where

$$\tilde{\boldsymbol{\xi}} = \begin{pmatrix} \xi_0 \\ \boldsymbol{\xi} \end{pmatrix}, \quad \tilde{E} = \begin{pmatrix} \eta_{00} & \boldsymbol{\eta}^T \\ \boldsymbol{\eta} & E \end{pmatrix}. \quad (25)$$

### 3. CP TRANSFORMATIONS AND CP INVARIANCE OF THE LAGRANGIAN

#### 3.1. The standard CP transformation

The standard CP transformation of the gauge fields and the Higgs fields reads (see for instance [26])

$$\begin{aligned}W^\mu(x) &\xrightarrow{\text{CP}_s} -W_\mu^T(x'), \\ B^\mu(x) &\xrightarrow{\text{CP}_s} -B_\mu(x'),\end{aligned}\quad (26)$$

$$\varphi_i(x) \xrightarrow{\text{CP}_s} \varphi_i^*(x') \quad (i = 1, 2). \quad (27)$$

Here we have

$$(x^\mu) = \begin{pmatrix} x^0 \\ \mathbf{x} \end{pmatrix}, \quad (x'^\mu) = \begin{pmatrix} x^0 \\ -\mathbf{x} \end{pmatrix} \quad (28)$$

and

$$W^\mu(x) = W^{\mu a}(x) \frac{1}{2} \tau_a \quad (29)$$

is the matrix of the  $W$ -potentials. Of course, a discussion of this CP transformation makes only sense once we have already chosen a particular basis for the two Higgs doublets since basis transformations (16) change (27). Such a particular choice of basis is, indeed, in general required when the Yukawa term  $\mathcal{L}_{\text{Yuk}}$  is taken into consideration. In the MSSM, for instance, one Higgs doublet couples to the up-type fermions, one to the down type fermions. This clearly singles out a special basis. Therefore, we have denoted the CP transformations in (26) and (27) by  $\text{CP}_s$  for *standard* and *special*.

From the definition of our matrix  $\underline{K}$  and of the four real coefficients  $K_0$  and  $K_a$  it is obvious that the  $\text{CP}_s$  transformations (27) correspond to

$$\begin{aligned} \underline{K}(x) &\xrightarrow{\text{CP}_s} \underline{K}^*(x') = \underline{K}^T(x'), \\ K_0(x) &\xrightarrow{\text{CP}_s} K_0(x'), \\ \begin{pmatrix} K_1(x) \\ K_2(x) \\ K_3(x) \end{pmatrix} &\xrightarrow{\text{CP}_s} \begin{pmatrix} K_1(x') \\ -K_2(x') \\ K_3(x') \end{pmatrix}. \end{aligned} \quad (30)$$

That is, the vector  $\mathbf{K}(x)$  is subjected to a reflection on the 1–3 plane and a change of argument  $x \rightarrow x'$ ,

$$\mathbf{K}(x) \xrightarrow{\text{CP}_s} R_2 \mathbf{K}(x'), \quad (31)$$

where

$$R_2 := \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (32)$$

The potential  $V$  (14) allows for  $\text{CP}_s$  as a symmetry if and only if it contains no terms linear in  $K_2$ . The kinetic term in the Higgs-Lagrangian (3) is invariant under  $\text{CP}_s$  as defined in (26), (27). Thus, we have the following theorem.

**Theorem 1.** *The Higgs Lagrangian (3) with the general potential (14) is invariant under the  $\text{CP}_s$  transformation (26), (27) if and only if*

$$\xi_2 = 0, \quad \eta_2 = 0, \quad \eta_{12} = \eta_{23} = 0. \quad (33)$$

Equivalently, we can formulate (33) with the help of the reflection matrix (32) as

$$R_2 \boldsymbol{\xi} = \boldsymbol{\xi}, \quad R_2 \boldsymbol{\eta} = \boldsymbol{\eta}, \quad R_2 E R_2^T = E. \quad (34)$$

### 3.2. Generalised CP transformations

We shall in this paper also consider *generalised* CP transformations of the Higgs fields [27] defined by

$$\varphi_i(x) \xrightarrow{\text{CP}_g} U_{\varphi, ij} \varphi_j^*(x'), \quad (35)$$

with  $i = 1, 2$  and  $U_\varphi = (U_{\varphi, ij}) \in U(2)$ . That is, the complex conjugation of the Higgs fields is supplemented by a basis transformation (16). The transformation of the gauge potentials stays the same as in (26),

$$\begin{aligned} W^\mu(x) &\xrightarrow{\text{CP}_g} -W_\mu^T(x'), \\ B^\mu(x) &\xrightarrow{\text{CP}_g} -B_\mu(x'). \end{aligned} \quad (36)$$

The  $\text{CP}_g$  transformation (35) implies for the gauge invariant functions (9) and (10)

$$\begin{aligned} \underline{K}(x) &\xrightarrow{\text{CP}_g} U_\varphi \underline{K}^*(x') U_\varphi^\dagger, \\ K_0(x) &\xrightarrow{\text{CP}_g} K_0(x'), \\ \mathbf{K}(x) &\xrightarrow{\text{CP}_g} R(U_\varphi) R_2 \mathbf{K}(x'), \end{aligned} \quad (37)$$

with  $R(U_\varphi) \in SO(3)$  obtained from (19) with  $U$  replaced by  $U_\varphi$ . That is,  $\text{CP}_g$  induces an *improper* rotation  $\bar{R}_\varphi$  of the vector  $\mathbf{K}$  in addition to the change of argument  $x \rightarrow x'$ :

$$\begin{aligned} K_0(x) &\xrightarrow{\text{CP}_g} K_0(x'), \\ \mathbf{K}(x) &\xrightarrow{\text{CP}_g} \bar{R}_\varphi \mathbf{K}(x'), \end{aligned} \quad (38)$$

where

$$\begin{aligned} \bar{R}_\varphi &= R(U_\varphi) R_2, \\ \bar{R}_\varphi \bar{R}_\varphi^T &= \mathbb{1}_3, \\ \det \bar{R}_\varphi &= \det (R(U_\varphi) R_2) = -1. \end{aligned} \quad (39)$$

From the results of section 2 it is clear that to any improper rotation  $\bar{R}_\varphi$  there is a  $U_\varphi \in U(2)$  which, inserted in (35), gives (38) and (39).

Thus, asking if the potential  $V$  (14) allows for a  $\text{CP}_g$  symmetry is the same as asking if it is invariant under some improper rotation (38) of the  $\mathbf{K}$ -vectors. That is, we have invariance under a  $\text{CP}_g$  transformation if the parameters of  $V$  (14) satisfy

$$\bar{R}_\varphi \boldsymbol{\xi} = \boldsymbol{\xi}, \quad \bar{R}_\varphi \boldsymbol{\eta} = \boldsymbol{\eta}, \quad \bar{R}_\varphi E \bar{R}_\varphi^T = E \quad (40)$$

for some improper rotation matrix  $\bar{R}_\varphi$ .

We shall study now the effect of a basis change (16) on  $\bar{R}_\varphi$ . For this it is convenient to work with the matrix  $\phi(x)$  (8). Let the new basis fields be  $\varphi'_1(x)$ ,  $\varphi'_2(x)$  and the corresponding matrix

$$\phi'(x) = \begin{pmatrix} \varphi'_1(x) & \varphi'_1(x) \\ \varphi'_2(x) & \varphi'_2(x) \end{pmatrix} = U \phi(x) \quad (41)$$

with  $U \in U(2)$ . The  $\text{CP}_g$  transformation (35) reads

$$\phi(x) \xrightarrow{\text{CP}_g} U_\varphi \phi^*(x'). \quad (42)$$

This implies

$$\begin{aligned} \phi'(x) &\xrightarrow{\text{CP}_g} UU_\varphi \phi^*(x') \\ &= UU_\varphi U^{*-1} \phi'^*(x') \\ &= U'_\varphi \phi'^*(x'), \end{aligned} \quad (43)$$

where

$$U'_\varphi = UU_\varphi U^{*-1}. \quad (44)$$

The transformation of  $K'_0(x)$  and  $\mathbf{K}'(x)$  in the new basis is

$$\begin{aligned} K'_0(x) &\xrightarrow{\text{CP}_g} K'_0(x'), \\ \mathbf{K}'(x) &\xrightarrow{\text{CP}_g} \bar{R}'_\varphi \mathbf{K}'(x'), \end{aligned} \quad (45)$$

with

$$\bar{R}'_\varphi = R(U'_\varphi) R_2 = R(U) \bar{R}_\varphi R^T(U). \quad (46)$$

Here  $R(U) \in SO(3)$  is the rotation matrix obtained from  $U$  according to (19). Thus, a basis change induces an orthogonal transformation of the improper rotation matrix  $\bar{R}_\varphi$ .

Now we shall consider two successive  $\text{CP}_g$  transformations. For the gauge potentials and for the gauge invariant functions we find from (36) and (38):

$$\begin{aligned} W^\mu(x) &\xrightarrow{\text{CP}_g \circ \text{CP}_g} W^\mu(x), \\ B^\mu(x) &\xrightarrow{\text{CP}_g \circ \text{CP}_g} B^\mu(x), \\ K_0(x) &\xrightarrow{\text{CP}_g \circ \text{CP}_g} K_0(x), \\ \mathbf{K}(x) &\xrightarrow{\text{CP}_g \circ \text{CP}_g} (\bar{R}_\varphi)^2 \mathbf{K}(x). \end{aligned} \quad (47)$$

Requiring that  $\text{CP}_g \circ \text{CP}_g$  gives the unit transformation for the gauge invariant functions leads to the condition

$$\bar{R}_\varphi \bar{R}_\varphi = \mathbb{1}_3. \quad (48)$$

But we also have  $\bar{R}_\varphi \bar{R}_\varphi^T = \mathbb{1}_3$ ; see (39). The requirement (48) thus means that  $\bar{R}_\varphi$  is symmetric

$$\bar{R}_\varphi^T = \bar{R}_\varphi. \quad (49)$$

As a real symmetric matrix it can be diagonalised by an orthogonal matrix  $R(U)$ . That is, we can make a basis change of the Higgs fields as in (41) and achieve

$$\bar{R}'_\varphi = R(U) \bar{R}_\varphi R^T(U) = \text{diagonal matrix}. \quad (50)$$

Since  $\bar{R}'_\varphi$  is an improper rotation it satisfies  $\bar{R}'_\varphi \bar{R}'_\varphi^T = \mathbb{1}_3$  and  $\det \bar{R}'_\varphi = -1$ . Thus, we have only the possibilities  $\bar{R}'_\varphi = R_1$  or  $R_2$  or  $R_3$  or  $-\mathbb{1}_3$ . Here

$$\begin{aligned} R_1 &:= \text{diag}(-1, 1, 1), \\ R_2 &:= \text{diag}(1, -1, 1), \\ R_3 &:= \text{diag}(1, 1, -1). \end{aligned} \quad (51)$$

The cases  $\bar{R}'_\varphi = R_j$ ,  $j = 1, 2, 3$  are equivalent by a basis change. Thus we find the following.

An improper rotation  $\bar{R}_\varphi$  satisfying  $\bar{R}_\varphi^2 = \mathbb{1}_3$  is either

$$(i) \quad \bar{R}_\varphi = -\mathbb{1}_3, \quad (52)$$

that is, a point reflection, or orthogonally equivalent to the reflection  $R_2$

$$(ii) \quad \bar{R}_\varphi = R^T(U) R_2 R(U), \quad (53)$$

that is, a reflection on a plane.

*CP<sub>g</sub> transformations of type (i)*

For the case (i),  $\bar{R}_\varphi$  as in (52), the  $\text{CP}_g$  transformation for the fields is obtained from (42) by setting  $U_\varphi = \epsilon$ ,

$$\phi(x) \xrightarrow{\text{CP}_g} \epsilon \phi^*(x'), \quad (54)$$

where  $\epsilon$  is defined in (6). With this we obtain indeed

$$\begin{aligned} \underline{K}(x) &\xrightarrow{\text{CP}_g} \epsilon \phi^*(x') \phi'^{\dagger}(x') \epsilon^T \\ &= \epsilon \underline{K}^T(x') \epsilon^T \\ &= \frac{1}{2} (K_0(x') \mathbb{1}_2 - \mathbf{K}(x') \boldsymbol{\sigma}), \\ \mathbf{K}(x) &\xrightarrow{\text{CP}_g} -\mathbf{K}(x'). \end{aligned} \quad (55)$$

Note that here  $\text{CP}_g \circ \text{CP}_g$  gives the unit transformation for the Higgs fields only after a suitable gauge transformation. We have

$$\phi(x) \xrightarrow{\text{CP}_g \circ \text{CP}_g} \epsilon (\epsilon \phi^*(x))^* = -\phi(x). \quad (56)$$

A hypercharge gauge transformation

$$U_G = \exp(2\pi i \mathbf{Y}) \quad (57)$$

with  $\mathbf{Y} = \frac{1}{2} \mathbb{1}_2$  for the Higgs fields gives (see (A.7) of [4])

$$\phi(x) \xrightarrow{U_G} \phi(x) U_G^T = \phi(x) (-1). \quad (58)$$

Thus, for the case (i), (52), the transformation

$$\exp(2\pi i \mathbf{Y}) \circ \text{CP}_g \circ \text{CP}_g \quad (59)$$

is the unit transformation for the Higgs fields and, as we easily check, also for the gauge potentials. In appendix B

we show that, up to gauge transformations, the transformation of the fields given in (54) is the only possible one giving a  $\text{CP}_g$  transformation of type (i). We also show there that (54) holds in *any* basis, again up to gauge transformations. Thus the  $\text{CP}_g$  transformations of type (i) have the very interesting, one might even say aesthetic, property of having the same form in any Higgs basis.

The invariance conditions for the potential parameters, (40), give us here the following theorem.

**Theorem 2.** *The Higgs boson Lagrangian (3) with the potential (14) has the  $\text{CP}_g$  symmetry (36), (38) of type (i), where  $\bar{R}_\varphi = -1_3$  (see (52)), if and only if*

$$\boldsymbol{\xi} = 0 \quad \text{and} \quad \boldsymbol{\eta} = 0. \quad (60)$$

We note that the statements of theorem 2 are basis independent, since the conditions  $\boldsymbol{\xi} = 0$  and  $\boldsymbol{\eta} = 0$  are not affected by a change of basis. This is a direct consequence of the basis independence of the form of the  $\text{CP}_g$  transformation of type (i).

#### $\text{CP}_g$ transformations of type (ii)

For the case (ii),  $\bar{R}_\varphi$  as in (53), we find that the original  $\text{CP}_g$  transformation (35) is equal to the standard  $\text{CP}_s$  transformation (27) for the Higgs fields after a suitable change of basis, see (16) and (41):

$$\varphi'_i(x) \xrightarrow{\text{CP}_g} \varphi'^*_i(x') \quad (i = 1, 2). \quad (61)$$

Using now the results of section 3.1 we find that the THDM potential (14) will be invariant under a  $\text{CP}_g$  transformation of type (ii) if and only if we can find a basis transformation (16) eliminating all odd powers of  $K_2$ . That is, there must exist some  $R(U) \in \text{SO}(3)$  such that

$$\begin{aligned} \boldsymbol{\xi}' &= R(U) \boldsymbol{\xi} = \begin{pmatrix} \cdot \\ 0 \\ \cdot \end{pmatrix}, \\ \boldsymbol{\eta}' &= R(U) \boldsymbol{\eta} = \begin{pmatrix} \cdot \\ 0 \\ \cdot \end{pmatrix}, \\ E' &= R(U) E R^T(U) = \begin{pmatrix} \cdot & 0 & \cdot \\ 0 & \cdot & 0 \\ \cdot & 0 & \cdot \end{pmatrix}, \end{aligned} \quad (62)$$

where the dots represent arbitrary entries. Note that the central entry of  $E'$ , that is  $E'_{22}$ , need not vanish, since it corresponds to a quadratic term in  $K_2$ . Obviously, the first two conditions correspond to a rotation of the vector cross product  $\boldsymbol{\xi} \times \boldsymbol{\eta}$  into the 2-direction which is always achievable by suitable rotations around the 1- and the 3-axis. It is advantageous to formulate the conditions (62) in a way independent of the chosen basis, so that no rotations of the original parameters have to be performed.

In the following we shall show that the conditions (62) are equivalent to a simple set of equations. We formulate this result as a theorem.

**Theorem 3.** *The THDM potential  $V$  (14) is invariant under a  $\text{CP}_g$  transformation (36), (38) of type (ii) (see (53)) if and only if the following set of equations holds:*

$$(\boldsymbol{\xi} \times \boldsymbol{\eta})^T E \boldsymbol{\xi} = 0, \quad (63)$$

$$(\boldsymbol{\xi} \times \boldsymbol{\eta})^T E \boldsymbol{\eta} = 0, \quad (64)$$

$$(\boldsymbol{\xi} \times (E \boldsymbol{\xi}))^T E^2 \boldsymbol{\xi} = 0, \quad (65)$$

$$(\boldsymbol{\eta} \times (E \boldsymbol{\eta}))^T E^2 \boldsymbol{\eta} = 0. \quad (66)$$

The conditions (65) and (66) are required for the case  $\boldsymbol{\xi} \times \boldsymbol{\eta} = 0$ , which leads to trivial equations for (63) and (64) and thus gives no constraints on the matrix  $E$ . By insertion of the explicit expressions (62) it is seen that they are sufficient to satisfy (63)-(66). The proof that (63)-(66) are also necessary conditions for (62) to hold is more lengthy and thus is postponed to the appendix A. Since (63)-(66) just express linear dependencies of three-vector type quantities via vanishing triple products, it is obvious that these conditions are rotationally invariant. They are therefore independent of the chosen basis, that is independent of transformations (21) of the parameters. Thus we have found very simple and basis independent conditions (63)-(66) which are satisfied if and only if the THDM Higgs potential allows for a  $\text{CP}_g$  symmetry of type (ii).

The conditions (63)-(66) are equivalent to (23)-(26) in [14] as well as to the conditions given in (A)-(B) in [15]. The proof in appendix A shows how a Higgs basis is constructed for which the potential is invariant under the standard CP transformation, provided (63)-(66) hold. In this basis the parameters of the potential with respect to the Higgs fields,  $V(\varphi_1, \varphi_2)$ , are real. Note that by construction the parameters of  $V(\tilde{\mathbf{K}})$  are always real, independent of its CP properties.

We remark that the conditions (63)-(66) guarantee that the potential has at least one  $\text{CP}_g$  invariance transformation. It is possible that a theory has more than one  $\text{CP}_g$  invariance transformation. A sufficient condition guaranteeing the uniqueness of the  $\text{CP}_g$  transformation is

$$\boldsymbol{\xi} \times \boldsymbol{\eta} \neq 0. \quad (67)$$

Then, clearly the only reflection symmetry one can have is on the plane spanned by  $\boldsymbol{\xi}$  and  $\boldsymbol{\eta}$ . In appendix C, table I, we give a classification of  $\text{CP}_g$  type (ii) invariant theories with respect to the number of independent  $\text{CP}_g$  transformations they allow.

An additional remark concerns the relation of type (i) and (ii) symmetries. From theorems 2 and 3 we see that a theory having the  $\text{CP}_g$  symmetry of type (i) is also invariant under - in fact, several -  $\text{CP}_g$  transformations of type (ii). This is further discussed in appendix C.

Eventually we note, that we have classified the  $\text{CP}_g$  properties of the THDM according to the Higgs potential, regardless of whether these symmetries are spontaneously broken or not. Such a classification of symmetries at the Lagrangian level is interesting by itself for several reasons: through symmetries the parameters of the theory can be restricted. Moreover, at high temperature one expects to see the full symmetries of the theory explicitly. In particular, the phase structure of the theory will depend crucially on these symmetries. Symmetries may also point the road to generalisations of the theory relevant at higher energy scales.

In the following section we study in detail the conditions for spontaneous breaking of these  $\text{CP}_g$  symmetries.

#### 4. SPONTANEOUS CP VIOLATION

If there is no CP transformation under which the potential is invariant, CP is broken *explicitly*. If the potential is invariant under a certain  $\text{CP}_g$  transformation but the vacuum expectation value does not respect this symmetry we have *spontaneous* violation of this  $\text{CP}_g$  symmetry. Note that a potential can be symmetric under several  $\text{CP}_g$  transformations where some may be conserved and some violated by the vacuum expectation value. Examples for this case are given below.

The stationary points of  $V$  (14) with the lowest potential value give the vacuum solutions for  $\tilde{\mathbf{K}}(x)$  (23) and for the fields. We denote the corresponding values by

$$\langle \varphi_i \rangle := \langle \varphi_i(x) \rangle = \begin{pmatrix} v_i^+ \\ v_i^0 \end{pmatrix} \quad (68)$$

with  $i = 1, 2$ . We get then for the vacuum expectation values of the matrices  $\phi$  (8) and  $\underline{K}$  (9):

$$\langle \phi \rangle := \langle \phi(x) \rangle = \begin{pmatrix} v_1^+ & v_1^0 \\ v_2^+ & v_2^0 \end{pmatrix}, \quad (69)$$

$$\underline{K} = \frac{1}{2}(K_0 \mathbb{1}_2 + \mathbf{K} \boldsymbol{\sigma}) = \langle \phi \rangle \langle \phi \rangle^\dagger. \quad (70)$$

Note that the gauge invariant functions are written with argument in this section as  $K_0(x)$ ,  $\mathbf{K}(x)$ , whereas the vacuum expectation values are written without argument,  $K_0$ ,  $\mathbf{K}$ . Of course, for an acceptable theory the physical vacuum must accomplish electroweak symmetry breaking (EWSB). That is, the gauge group  $SU(2)_L \times U(1)_Y$  must be broken down to  $U(1)_{em}$ . In [4] it has been shown that this requires

$$K_0 = |\mathbf{K}| > 0. \quad (71)$$

That is, the vacuum solution for the Higgs fields must correspond to a non-zero light-like four-vector  $\tilde{\mathbf{K}}$ . This four-vector  $\tilde{\mathbf{K}}$  satisfies the stationarity condition (see (96) and (145) of [4] and (24) and (25))

$$\tilde{\boldsymbol{\xi}} = -2 \left( \tilde{E} - u_0 \tilde{g} \right) \tilde{\mathbf{K}}, \quad u_0 = \frac{m_{H^\pm}^2}{2v_0^2}, \quad (72)$$

where

$$\tilde{g} := \text{diag}(1, -1, -1, -1), \quad (73)$$

or written out in components

$$\xi_0 = -2(\eta_{00}K_0 - \frac{m_{H^\pm}^2}{2v_0^2}K_0 + \boldsymbol{\eta}^T \mathbf{K}), \quad (74)$$

$$\boldsymbol{\xi} = -2(E\mathbf{K} + \frac{m_{H^\pm}^2}{2v_0^2}\mathbf{K} + K_0\boldsymbol{\eta}). \quad (75)$$

Here  $m_{H^\pm}$  is the mass of the charged Higgs bosons and

$$v_0 \approx 246 \text{ GeV} \quad (76)$$

is the standard Higgs vacuum expectation value.

Suppose now that the potential  $V$  has a  $\text{CP}_g$  symmetry, that is, an invariance under an improper rotation  $\bar{R}_\varphi$ . The potential parameters satisfy then (40). This symmetry is spontaneously broken if and only if the vacuum expectation value  $\mathbf{K}$  does not respect this symmetry, that is, fulfills

$$\bar{R}_\varphi \mathbf{K} \neq \mathbf{K}. \quad (77)$$

Note the gauge invariance and basis independence of this condition.

We shall now study the  $\text{CP}_g$  transformations of the cases (i) and (ii) separately and discuss then the standard transformation  $\text{CP}_s$ .

##### 4.1. $\text{CP}_g$ invariance of type (i)

According to theorem 2 the potential having  $\text{CP}_g$  invariance of type (i) has the form (see (60))

$$V = \xi_0 K_0(x) + \eta_{00} K_0(x)^2 + \mathbf{K}(x)^T E \mathbf{K}(x). \quad (78)$$

From (71) we see that the correct EWSB requires  $\mathbf{K} \neq 0$ . This implies then (77) with  $\bar{R}_\varphi = -\mathbb{1}_3$ . That is, we have

$$-\mathbb{1}_3 \mathbf{K} \neq \mathbf{K}. \quad (79)$$

We formulate this result as a theorem:

**Theorem 4.** *A theory which is invariant under the  $\text{CP}_g$  type (i) transformation has the potential (78). The required EWSB implies that the  $\text{CP}_g$  type (i) symmetry is spontaneously broken.*

In appendix B we discuss in detail the stability and EWSB properties of this class of models having the potential (78). There we prove the following theorem.

**Theorem 5.** *Consider the Higgs part of the THDM Lagrangian (3) with the potential (78) having  $\text{CP}_g$  invariance of type (i). Let  $\mu_1 \geq \mu_2 \geq \mu_3$  be the eigenvalues of  $E$  with this ordering. The theory is stable, has the correct*

*EWSB and no zero mass charged Higgs boson if and only if*

$$\begin{aligned} \eta_{00} &> 0, \\ \mu_a + \eta_{00} &> 0 \quad \text{for } a = 1, 2, 3, \\ \xi_0 &< 0, \\ \mu_3 &< 0. \end{aligned} \quad (80)$$

*The  $\text{CP}_g$  symmetry of type (i) is then spontaneously broken.*

This clarifies the case of THDM models with type (i)  $\text{CP}_g$  symmetry completely.

#### 4.2. $\text{CP}_g$ invariance of type (ii)

For a theory having a  $\text{CP}_g$  invariance of type (ii) the parameters of the potential  $V$  must satisfy (63)-(66) according to theorem 3. Such a  $\text{CP}_g$  symmetry is spontaneously broken if (77) holds with  $\bar{R}_\varphi$  as in (53). Suppose now that for given parameters satisfying (63)-(66) it has been checked that  $V$  is a stable potential. Suppose furthermore, that the vacuum solution  $\underline{K}$  (70) has been identified. For this we can use, for instance, the methods of [4]. The following theorem allows us then to check if  $\text{CP}_g$  is spontaneously violated or not.

**Theorem 6.** *Suppose that the potential is invariant under one or more  $\text{CP}_g$  type (ii) transformations, that is, its parameters respect (63)-(66). Let  $K_0, \mathbf{K}$  be the vacuum solution. The question if there is a  $\text{CP}_g$  invariance which is also respected by the vacuum can be decided by checking the following three relations:*

$$(\boldsymbol{\xi} \times \boldsymbol{\eta})^T \mathbf{K} = 0, \quad (81)$$

$$(\boldsymbol{\xi} \times (E\boldsymbol{\xi}))^T \mathbf{K} = 0, \quad (82)$$

$$(\boldsymbol{\eta} \times (E\boldsymbol{\eta}))^T \mathbf{K} = 0. \quad (83)$$

We distinguish two cases.

$$(a) \quad \boldsymbol{\xi} \times \boldsymbol{\eta} \neq 0.$$

*The theory allows then exactly for one  $\text{CP}_g$  type (ii) invariance transformation which is conserved also by the vacuum if and only if (81) holds. In this case (82) and (83) are a consequence of (81).*

$$(b) \quad \boldsymbol{\xi} \times \boldsymbol{\eta} = 0.$$

*Then (81) is trivial. There may be more than one  $\text{CP}_g$  type (ii) invariance transformation. At least one of these symmetries is also respected by the vacuum if (82) and (83) hold.*

The proof of theorem 6 is presented in appendix C. We find that the conditions (81)-(83) for the absence of spontaneous CP violation are equivalent to the conditions given in theorem 4 of [14], which were proven in

[13] and found before in [11, 12]. We find that the criteria a)-c) in [15] correspond to (81)-(82) and should be supplemented by (83) to cover the fully general case. We give the details in appendix C.

We emphasise that the formulation *absence of spontaneous CP violation* is not quite appropriate in this context. The correct statement is given in theorem 6 above. It covers also the case that the theory has more than one independent  $\text{CP}_g$  type (ii) invariance transformation where one is respected by the vacuum and another spontaneously broken. These *mixed* cases in fact occur; see appendix C.

As discussed in the previous subsection, a type (i) symmetry is necessarily spontaneously broken in an acceptable theory. On the other hand, a type (i) symmetric model has at least three type (ii) symmetries. It is straightforward to verify that the vacuum respects at least one of these symmetries; see appendix C.

To check the conditions (81)-(83) we have to know the vacuum expectation value  $\tilde{\mathbf{K}}$ . In theorem 2 of [4] a classification of all stationary solutions as type (Ia) to (III) has been given, covering in particular the vacuum solution. We discuss in appendix D two necessary conditions for the occurrence of spontaneous breaking of a  $\text{CP}_g$  type (ii) invariance. We formulate this as a theorem.

**Theorem 7.** *Spontaneous breaking of a  $\text{CP}_g$  type (ii) invariance can only occur if the vacuum solution is of type (IIb) (see theorem 2 of [4]). That is, the vacuum value  $\tilde{\mathbf{K}}$  must be a solution of (72) where*

$$\det(\tilde{E} - u_0 \tilde{g}) = 0. \quad (84)$$

*Furthermore, in the basis (62) we must have*

$$\eta'_{22} = -u_0 = -\frac{m_{H^\pm}^2}{2v_0^2} < 0 \quad (85)$$

*if the  $\text{CP}_g$  symmetry, corresponding to the reflection  $R_2$  (32) in this basis, is spontaneously broken.*

#### 4.3. $\text{CP}_s$ invariance

This is, of course, a special case of  $\text{CP}_g$  invariance of type (ii). But now it is convenient to discuss the situation with respect to the distinguished basis where the CP transformation is of the standard type (see (30), (31)),

$$\begin{aligned} K_0(x) &\xrightarrow{\text{CP}_s} K_0(x'), \\ \mathbf{K}(x) &\xrightarrow{\text{CP}_s} R_2 \mathbf{K}(x'), \end{aligned} \quad (86)$$

with  $R_2$  the reflection on the 1-3 plane, see (32). Spontaneous  $\text{CP}_s$  violation means in this basis, from (77) with  $\bar{R}_\varphi = R_2$ , that the vacuum does not respect this symmetry:

$$R_2 \mathbf{K} \neq \mathbf{K}, \quad (87)$$



that is, we have

$$K_2 \neq 0. \quad (88)$$

An acceptable theory must have a physical vacuum which breaks  $SU(2)_L \times U(1)_Y$  down to  $U(1)_{em}$ . In this case the vacuum expectation values of the Higgs doublets may be parametrised by

$$\langle \varphi_1 \rangle = \begin{pmatrix} 0 \\ v_1 \end{pmatrix}, \quad \langle \varphi_2 \rangle = \begin{pmatrix} 0 \\ v_2 e^{i\zeta} \end{pmatrix}. \quad (89)$$

Here  $v_1, v_2, \zeta$  are real numbers with  $v_1 \geq 0$ ,  $v_2 \geq 0$ ,  $-\pi < \zeta \leq \pi$ , and a possible phase of  $\langle \varphi_1 \rangle$  has been eliminated by a  $U(1)_Y$  gauge transformation. The standard Higgs vacuum expectation value is

$$v_0 = \sqrt{2(v_1^2 + v_2^2)} \approx 246 \text{ GeV}. \quad (90)$$

For  $v_1 \neq 0$  the usual mixing parameter  $\tan \beta$  can be defined as  $\tan \beta := v_2/v_1$  with  $0 \leq \beta < \pi/2$ . The vacuum expectation values of the gauge invariant functions are determined from (68)-(70) with (89) as

$$\tilde{\mathbf{K}} = \begin{pmatrix} v_1^2 + v_2^2 \\ 2v_1 v_2 \cos \zeta \\ 2v_1 v_2 \sin \zeta \\ v_1^2 - v_2^2 \end{pmatrix}. \quad (91)$$

From (88) we find the well known result that  $CP_s$  is violated spontaneously if and only if  $v_1 \neq 0$ ,  $v_2 \neq 0$ ,  $\zeta \neq 0$  or  $\pi$ . That is, the vacuum expectation values of the two Higgs fields in this special basis must be complex relative to each other. We note, however, that this statement has no basis-independent meaning. Concerning a detailed discussion of this point see also [16]. By a suitable basis transformation we can always achieve that only one Higgs doublet has a non-vanishing vacuum expectation value which, moreover, is real. See chapter 6 of [4].

At the end of this chapter we make some general remarks concerning the parameters of the THDM potential (see (14), (24)). From (72) it looks tempting to replace  $\tilde{\xi}$  by the stationarity condition with  $\tilde{\mathbf{K}}$  given in (91) (and  $v_1$  eliminated by means of (90)):

$$\tilde{\xi} = \tilde{\xi}(v_0, v_2, \zeta, m_{H^\pm}, \eta_{00}, \boldsymbol{\eta}, E). \quad (92)$$

With this the potential can be reparametrised in terms of  $v_0, v_2, \zeta, m_{H^\pm}, \eta_{00}, \boldsymbol{\eta}, E$ . With this set of independent input parameters,  $v_0$  can be adjusted to the required value (90), and relations involving the vacuum solution, such as the CP invariance conditions (63)-(66), can be evaluated directly in terms of input parameters. Note, that this parametrisation (92) is possible for all potentials having a non-zero stationary point  $\tilde{\mathbf{K}}$  on the light cone. A potential not having such a point can not have the required EWSB behaviour. After the substitution (92) the four-vector  $\tilde{\mathbf{K}}$  in (91) corresponds by construction to a stationary point of  $V$ . Thus, the parametrisation (92) is

possible for all potentials with a stationary point at the wanted place (91). But for any concrete values of the new parameters it remains to be checked whether  $\tilde{\mathbf{K}}$  in (91) is indeed the global minimum of a stable potential  $V$ . This typically requires to make the complete analysis of stability and EWSB for  $V$ , for instance with the methods of [4]. Note that in the gauge invariant function approach this change of parameters is even possible for the cases where the phase  $\zeta$  or one of  $v_1, v_2$  vanishes.

## 5. EXAMPLES

Here we apply the general considerations of Sections 3 and 4 to specific models.

### 5.1. CP symmetric model with $\xi = \eta = 0$

We consider the THDM with the Higgs potential

$$\begin{aligned} V(\varphi_1, \varphi_2) = & m_{11}^2 \left( \varphi_1^\dagger \varphi_1 + \varphi_2^\dagger \varphi_2 \right) \\ & + \frac{1}{2} \lambda_1 \left( (\varphi_1^\dagger \varphi_1)^2 + (\varphi_2^\dagger \varphi_2)^2 \right) \\ & + \lambda_3 (\varphi_1^\dagger \varphi_1) (\varphi_2^\dagger \varphi_2) + \lambda_4 (\varphi_1^\dagger \varphi_2) (\varphi_2^\dagger \varphi_1) \\ & + \frac{1}{2} \lambda_5 \left( (\varphi_1^\dagger \varphi_2)^2 + (\varphi_2^\dagger \varphi_1)^2 \right), \end{aligned} \quad (93)$$

where all parameters are real. This potential is invariant under  $\varphi_1 \rightarrow -\varphi_1$ . We put the potential into the form (14) using the relations (11). Then,

$$\begin{aligned} \eta_{00} &= \frac{1}{4}(\lambda_1 + \lambda_3), \\ \boldsymbol{\eta} &= \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \\ E &= \frac{1}{4} \begin{pmatrix} \lambda_4 + \lambda_5 & 0 & 0 \\ 0 & \lambda_4 - \lambda_5 & 0 \\ 0 & 0 & \lambda_1 - \lambda_3 \end{pmatrix}, \\ \xi_0 &= m_{11}^2, \\ \boldsymbol{\xi} &= \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}. \end{aligned} \quad (94)$$

Obviously this model fulfills the conditions of theorem 2, that is, has a  $CP_g$  symmetry of type (i). Furthermore, the potential has at least three  $CP_g$  symmetries of type (ii), namely  $R_1, R_2, R_3$ , and infinitely many if two or three eigenvalues of  $E$  coincide. Note that the condition  $\boldsymbol{\xi} = \boldsymbol{\eta} = 0$  is basis independent. This in turn means that every potential with  $\boldsymbol{\xi} = \boldsymbol{\eta} = 0$  can be cast into the form (93) respectively (94) with an appropriate basis transformation.

We see from theorem 5 and the discussion in appendix B that this model is stable *in the strong sense* if simultaneously  $\lambda_1 > 0$ ,  $\lambda_1 + \lambda_3 > 0$  and  $\lambda_1 + \lambda_3 + \lambda_4 > |\lambda_5|$ .

Moreover, it has the right electroweak symmetry breaking behaviour for  $\xi_0 < 0$  or equivalently  $m_{11}^2 < 0$ . In the case of  $m_{11}^2 < 0$  the  $\text{CP}_g$  symmetry of type (i) is spontaneously broken. However, at least one  $\text{CP}_g$  symmetry of type (ii) is respected by the vacuum; see also appendix C.

## 5.2. CP properties of the “almost general” THDM

We consider a class of THDMs with the Higgs potential

$$\begin{aligned} V(\varphi_1, \varphi_2) = & m_{11}^2 \varphi_1^\dagger \varphi_1 + m_{22}^2 \varphi_2^\dagger \varphi_2 \\ & - \left[ m_{12}^2 \varphi_1^\dagger \varphi_2 + h.c. \right] \\ & + \frac{1}{2} \lambda_1 (\varphi_1^\dagger \varphi_1)^2 + \frac{1}{2} \lambda_2 (\varphi_2^\dagger \varphi_2)^2 \\ & + \lambda_3 (\varphi_1^\dagger \varphi_1) (\varphi_2^\dagger \varphi_2) + \lambda_4 (\varphi_1^\dagger \varphi_2) (\varphi_2^\dagger \varphi_1) \\ & + \left[ \frac{1}{2} \lambda_5 (\varphi_1^\dagger \varphi_2)^2 + h.c. \right], \end{aligned} \quad (95)$$

written in the parametrisation of [24], where  $m_{12}^2$  and  $\lambda_5$  may be arbitrary complex and all other parameters are real. This potential breaks the discrete symmetry  $\varphi_1 \rightarrow -\varphi_1$  only softly, that is by quadratic terms in the Higgs doublet fields, thus suppressing large flavour-changing neutral currents. We put the potential into the form (14) using the relations (11) and get here

$$\begin{aligned} \eta_{00} &= \frac{1}{8}(\lambda_1 + \lambda_2 + 2\lambda_3), \\ \boldsymbol{\eta} &= \frac{1}{8} \begin{pmatrix} 0 \\ 0 \\ \lambda_1 - \lambda_2 \end{pmatrix}, \\ E &= \frac{1}{4} \begin{pmatrix} \lambda_4 + \text{Re } \lambda_5 & -\text{Im } \lambda_5 & 0 \\ -\text{Im } \lambda_5 & \lambda_4 - \text{Re } \lambda_5 & 0 \\ 0 & 0 & \frac{1}{2}(\lambda_1 + \lambda_2 - 2\lambda_3) \end{pmatrix}, \\ \xi_0 &= \frac{1}{2}(m_{11}^2 + m_{22}^2), \\ \boldsymbol{\xi} &= \begin{pmatrix} -\text{Re } m_{12}^2 \\ \text{Im } m_{12}^2 \\ \frac{1}{2}(m_{11}^2 - m_{22}^2) \end{pmatrix}. \end{aligned} \quad (96)$$

The stability of the potential is easily investigated using the methods of [4]. Stability is guaranteed by the terms quartic in the fields alone if and only if

$$\lambda_1 > 0, \quad \lambda_2 > 0, \quad \text{and } \sqrt{\lambda_1 \lambda_2} + \lambda_3 > \max(0, |\lambda_5| - \lambda_4). \quad (97)$$

In order to determine the CP properties of the potential we have to check (63)-(66). Two of the conditions for  $\text{CP}_g$  type (ii) invariance of the potential, (64) and (66),

are, with (96), automatically fulfilled. The remaining conditions (63) and (65) give

$$(\lambda_1 - \lambda_2) \text{Im}((m_{12}^2)^2 \lambda_5^*) = 0, \quad (98)$$

$$\begin{aligned} & \left[ (\lambda_1 + \lambda_2 - 2(\lambda_3 + \lambda_4))^2 - 4|\lambda_5|^2 \right] \\ & \times (m_{11}^2 - m_{22}^2) \text{Im}((m_{12}^2)^2 \lambda_5^*) = 0 \end{aligned} \quad (99)$$

as necessary and sufficient conditions for the existence of a  $\text{CP}_g$  invariance of type (ii) for the potential. It is obvious that for the case of real parameters  $m_{12}^2$  and  $\lambda_5$  (98) and (99) are satisfied. For  $\boldsymbol{\xi} \times \boldsymbol{\eta}$  we find from (96)

$$\boldsymbol{\xi} \times \boldsymbol{\eta} = \frac{1}{8}(\lambda_1 - \lambda_2) \begin{pmatrix} \text{Im}(m_{12}^2) \\ \text{Re}(m_{12}^2) \\ 0 \end{pmatrix}. \quad (100)$$

From theorem 3 ff. we find, therefore, that in this model the potential allows one or more  $\text{CP}_g$  symmetries if and only if (98) and (99) hold. There is exactly one  $\text{CP}_g$  symmetry if  $\lambda_1 - \lambda_2 \neq 0$  and  $m_{12}^2 \neq 0$ .

In the case  $\text{CP}_g$  is conserved, that is (98), (99) are fulfilled,  $\text{CP}_g$  may be violated spontaneously. We reparametrise the potential using the stationarity conditions (74), (75) and assume that the vacuum expectation values  $v_1, v_2$  together with the phase  $\zeta$  indeed describe the global minimum (91) of the potential. We check the conditions for spontaneous  $\text{CP}_g$  violation (81)-(83) and see that (83) is automatically fulfilled. We find that (81) and (82) together with (98) and (99) are equivalent to the condition that either

$$v_1 v_2 [\cos(2\zeta) \text{Im } \lambda_5 + \sin(2\zeta) \text{Re } \lambda_5] = 0 \quad (101)$$

or

$$\lambda_1 = \lambda_2, \quad (v_1^2 - v_2^2) [(\lambda_3 + \lambda_4 - \lambda_1)^2 - |\lambda_5|^2] = 0 \quad (102)$$

or both are fulfilled. That is, exactly if (101) or (102) or both are fulfilled, there is a  $\text{CP}_g$  symmetry of both the potential and the vacuum expectation value  $\vec{\mathbf{K}}$ .

## 6. CONCLUSIONS

In this work we have shown that the framework of gauge invariant functions is well suited to discuss CP properties of the general THDM. These real gauge invariant functions build a four-vector for which we could reveal a simple geometric picture: Mixing of the two Higgs doublets corresponds to rotations and CP transformations to reflections of the *space-like* components of this four-vector.

In this geometric picture we have first given a classification of possible CP transformations in the THDM; see section 3. The standard CP transformation involves no mixing of the two doublet fields and corresponds to a reflection on the 1-3 plane. We identified two types, (i)

and (ii), of generalised CP transformations where arbitrary unitary mixing of the two doublet fields is allowed. The type (i)  $\text{CP}_g$  transformation is represented by a point reflection and has, to our knowledge, not been discussed before. We gave conditions for a theory to be symmetric under this transformation in theorem 2. Type (ii)  $\text{CP}_g$  transformations correspond to reflections on planes and include in particular the standard CP transformation. In theorem 3 we gave simple and easy to check conditions the parameters of the THDM potential have to satisfy if the Higgs Lagrangian is to be invariant under a  $\text{CP}_g$  transformation. We also gave a classification showing which THDMs allow for just one  $\text{CP}_g$  symmetry and which for more than one; see table I in appendix C.

In section 4 we turned to the question whether in a CP symmetric theory the vacuum respects the symmetry or not. We derived necessary and sufficient conditions for this to be the case. Again, the conditions to be checked are in all cases simple and have a transparent geometric meaning. See theorems 4-7 and (87), (88). We emphasise that a THDM can have more than one  $\text{CP}_g$  invariance where one may be spontaneously broken while another is conserved by the vacuum. This is again a crucial element for the discussions in the companion paper [23].

In section 5 we have illustrated our geometric methods with two examples, namely the most general model respecting the  $\text{CP}_g$  type (i) symmetry, as well as a model where large flavour-changing neutral currents are suppressed.

We compared our results with the literature for cases where this is possible. Concerning the existence of a CP type (ii) symmetry, our results fully agree with those of [13, 14], where a completely different approach was used. For the existence of a CP type (ii) symmetry of the potential we agree with [15]. But our criteria for CP invariance of the vacuum give important supplements to those presented in [15].

As mentioned above we have introduced and discussed in our present paper as completely new element the  $\text{CP}_g$  symmetry of type (i). Furthermore we have given a thorough discussion of the cases where multiple  $\text{CP}_g$  transformations are allowed by the theory. All these new elements are essential ingredients for our companion paper [23].

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### APPENDIX A: BASIS INDEPENDENT CONDITIONS FOR $\text{CP}_g$ TYPE (ii) INVARIANCE OF THE POTENTIAL

In this appendix we complete the proof of theorem 3 by showing that the existence of a basis (62), meaning

$\text{CP}_g$  type (ii) invariance of the potential (see (53)), is equivalent to (63)-(66).

We show first that (62) implies (63)-(66). Indeed we have for  $\xi', \eta'$  and  $E'$  as in (62)

$$\begin{aligned}\xi' \times \eta' &= \begin{pmatrix} 0 \\ \cdot \\ 0 \end{pmatrix}, \\ E'\xi' &= \begin{pmatrix} \cdot \\ 0 \\ \cdot \end{pmatrix}, & E'\eta' &= \begin{pmatrix} \cdot \\ 0 \\ \cdot \end{pmatrix}, \\ \xi' \times E'\xi' &= \begin{pmatrix} 0 \\ \cdot \\ 0 \end{pmatrix}, & \eta' \times E'\eta' &= \begin{pmatrix} 0 \\ \cdot \\ 0 \end{pmatrix}.\end{aligned}\quad (\text{A.1})$$

Furthermore, for any vector  $\zeta_\perp$  with 2-component zero,

$$\zeta_\perp = \begin{pmatrix} \cdot \\ 0 \\ \cdot \end{pmatrix}, \quad (\text{A.2})$$

we have

$$E'\zeta_\perp = \begin{pmatrix} \cdot \\ 0 \\ \cdot \end{pmatrix}. \quad (\text{A.3})$$

Thus, for all vectors  $\zeta_\parallel$  of the form

$$\zeta_\parallel = \begin{pmatrix} 0 \\ \cdot \\ 0 \end{pmatrix} \quad (\text{A.4})$$

we have

$$\zeta_\parallel^T E' \zeta_\perp = 0. \quad (\text{A.5})$$

All expressions (63)-(66) are of the form (A.5) if (62) holds. The conditions are formulated in a rotationally invariant form. Thus, they hold for  $\xi, \eta, E$  if they hold for  $\xi', \eta', E'$ , q.e.d.

Now we want to show that from (63)-(66) follows (62) with a suitable rotation  $R(U)$ . First we choose a basis where

$$\begin{aligned}\xi' &= R(U) \xi = \begin{pmatrix} 0 \\ 0 \\ \xi'_3 \end{pmatrix}, \\ \eta' &= R(U) \eta = \begin{pmatrix} \eta'_1 \\ 0 \\ \eta'_3 \end{pmatrix}.\end{aligned}\quad (\text{A.6})$$

Note that there is always a rotation into this basis possible for two vectors. It remains to be shown that in addition  $\eta'_{12} = \eta'_{23} = 0$  can be achieved if (63)-(66) hold. We remark that  $E$  is a symmetric matrix (see (14)) and this property is not altered by a similarity transformation (21). We have to consider different cases depending

on whether the vector cross product

$$\boldsymbol{\xi}' \times \boldsymbol{\eta}' = \begin{pmatrix} 0 \\ \xi'_3 \eta'_1 \\ 0 \end{pmatrix} \quad (\text{A.7})$$

vanishes or not. Let us first assume that the vector cross product (A.7) does not vanish, that is, we have  $\xi'_3 \eta'_1 \neq 0$ . From (63) we find now

$$(\boldsymbol{\xi}' \times \boldsymbol{\eta}')^T E' \boldsymbol{\xi}' = \eta'_{23} \xi'^2_3 \eta'_1 = 0. \quad (\text{A.8})$$

This means that  $\eta'_{23} = \eta'_{32} = 0$ . Then (64) gives

$$(\boldsymbol{\xi}' \times \boldsymbol{\eta}')^T E' \boldsymbol{\eta}' = \eta'_{21} \xi'_3 \eta'^2_1 = 0, \quad (\text{A.9})$$

that is, we have also  $\eta'_{21} = \eta'_{12} = 0$ . Thus, the explicit form (62) follows from (63)-(66) for this case.

Now we have to consider also the special case of a vanishing vector cross product (A.7). In this case (63) and (64) are trivially fulfilled and give no constraint for the matrix  $E'$ . We shall now use (65) and (66) to prove (62). If  $\boldsymbol{\xi} \times \boldsymbol{\eta} = 0$  and  $\boldsymbol{\xi} = 0$  and  $\boldsymbol{\eta} = 0$  we can achieve (62) trivially by diagonalising  $E$ . Thus, consider the case that  $\boldsymbol{\xi} \times \boldsymbol{\eta} = 0$  and  $\boldsymbol{\xi} \neq 0$ . By an orthogonal transformation we can diagonalise  $E$ :

$$R(U_1)ER^T(U_1) = E' = \text{diag}(\mu_1, \mu_2, \mu_3). \quad (\text{A.10})$$

We get then in this basis already  $\eta'_{12} = \eta'_{23} = 0$ . Furthermore, we have

$$\begin{aligned} \boldsymbol{\xi}' &= \begin{pmatrix} \xi'_1 \\ \xi'_2 \\ \xi'_3 \end{pmatrix}, & E' \boldsymbol{\xi}' &= \begin{pmatrix} \mu_1 \xi'_1 \\ \mu_2 \xi'_2 \\ \mu_3 \xi'_3 \end{pmatrix}, \\ \boldsymbol{\xi}' \times E' \boldsymbol{\xi}' &= \begin{pmatrix} (\mu_3 - \mu_2) \xi'_2 \xi'_3 \\ (\mu_1 - \mu_3) \xi'_3 \xi'_1 \\ (\mu_2 - \mu_1) \xi'_1 \xi'_2 \end{pmatrix}, \end{aligned} \quad (\text{A.11})$$

and from (65),

$$\begin{aligned} (\boldsymbol{\xi}' \times (E' \boldsymbol{\xi}'))^T E'^2 \boldsymbol{\xi}' &= \\ (\mu_1 - \mu_2)(\mu_2 - \mu_3)(\mu_3 - \mu_1) \xi'_1 \xi'_2 \xi'_3 &= 0. \end{aligned} \quad (\text{A.12})$$

If all eigenvalues  $\mu_a$  are different we find from (A.12) that at least one  $\xi'_a$  must be zero. By a change of basis which interchanges the components we can achieve  $\xi'_2 = 0$  without introducing off-diagonal elements in  $E'$ . Then  $\boldsymbol{\eta}'$  being parallel to  $\boldsymbol{\xi}'$  implies  $\eta'_2 = 0$  and we found a basis of the form (62). Suppose, on the other hand, that at least two eigenvalues  $\mu_a$  are equal. Without loss of generality we can suppose

$$\mu_1 = \mu_2. \quad (\text{A.13})$$

By a rotation around the 3-axis, leaving  $E'$  diagonal, we can then achieve

$$\boldsymbol{\xi}' = \begin{pmatrix} \xi'_1 \\ 0 \\ \xi'_3 \end{pmatrix} \quad (\text{A.14})$$

and also  $\eta'_2 = 0$  since  $\boldsymbol{\eta}'$  is parallel to  $\boldsymbol{\xi}'$ , q.e.d. For the case  $\boldsymbol{\xi} \times \boldsymbol{\eta} = 0$  and  $\boldsymbol{\eta} \neq 0$  the argumentation runs along the same lines using (66) instead of (65). This completes the proof that the set of the conditions (63)-(66) is equivalent to the existence of a basis satisfying (62).

We compared our conditions (63)-(66) for CP invariance of the potential with (23)-(26) in [14]. In [14] the conditions were found by a systematic survey of all possible complex invariants - and there is an enormous number of such invariants - within a field based formulation, that is, in a completely different way. Our triple products required to vanish in (63), (64), and (66) turn out to be equal to  $-2^{-5} I_{2Y2Z}$ ,  $2^{-7} I_{Y3Z}$ , and  $-2^{-13} I_{6Z}$  in their notation. Despite the fact, that the fourth invariant occurring in [14] and our condition (65) are different, we can show that the full sets of conditions are equivalent. This is conveniently done by computing the *reduced Groebner bases* for both sets which are indeed equal (for a brief introduction to the formalism of Groebner bases see the appendix of [28]).

## APPENDIX B: THEORIES WITH CP<sub>g</sub> TYPE (i) INVARIANCE

Here we study the theories having a CP<sub>g</sub> invariance of type (i) in detail; see theorem 2, (60). The corresponding potential is given in (78).

We show first that the transformation (54) of the fields is unique, up to gauge transformations, in giving the CP<sub>g</sub> type (i) transformation for the gauge invariant functions:

$$\begin{aligned} K_0(x) &\rightarrow K_0(x'), \\ \mathbf{K}(x) &\rightarrow -\mathbf{K}(x'). \end{aligned} \quad (\text{B.1})$$

To see this we try to generalise (54) by setting

$$\phi(x) \xrightarrow{\text{CP}_g} V \epsilon \phi^*(x') \quad (\text{B.2})$$

with  $V \in U(2)$ . Every  $V \in U(2)$  can be represented as

$$V = e^{i\gamma} \tilde{V} \quad (\text{B.3})$$

with  $\gamma$  real and  $\tilde{V} \in SU(2)$ . The transformation of  $\underline{K}(x)$  and  $K_0(x)$ ,  $\mathbf{K}(x)$  induced by (B.2) reads (see (37) and (55))

$$\begin{aligned} \underline{K}(x) &\xrightarrow{\text{CP}_g} V \epsilon \underline{K}^T(x') \epsilon^T V^\dagger \\ &= \tilde{V} \epsilon \underline{K}^T(x') \epsilon^T \tilde{V}^\dagger \\ &= \tilde{V} \frac{1}{2} (K_0(x') \mathbb{1}_2 - \mathbf{K}(x') \boldsymbol{\sigma}) \tilde{V}^\dagger, \end{aligned} \quad (\text{B.4})$$

$$\begin{aligned} K_0(x) &\xrightarrow{\text{CP}_g} K_0(x'), \\ \mathbf{K}(x) &\xrightarrow{\text{CP}_g} -R(\tilde{V}) \mathbf{K}(x'). \end{aligned} \quad (\text{B.5})$$

Here  $R(\tilde{V})$  is obtained from (19) with  $U$  replaced by  $\tilde{V}$ . In order to obtain the  $\text{CP}_g$  transformation of type (i) from (B.5) we must have

$$R(\tilde{V}) = \mathbb{1}_3. \quad (\text{B.6})$$

which implies

$$\tilde{V} = \pm \mathbb{1}_2 \quad (\text{B.7})$$

since  $\tilde{V} \in SU(2)$ . From (B.2) and (B.3) we get, therefore, as the only possible transformations of the fields leading to a  $\text{CP}_g$  transformation of type (i)

$$\phi(x) \rightarrow e^{i\gamma} \epsilon \phi^*(x'), \quad (\text{B.8})$$

where in the case  $\tilde{V} = -\mathbb{1}_2$  we have redefined  $\gamma$  as  $\gamma + \pi$ . Both Higgs doublets have weak hypercharge  $y = +1/2$ . Thus a gauge transformation  $U_G \equiv \exp(-2i\gamma \mathbf{Y})$  brings back (B.8) to the form (54)

$$\phi(x) \xrightarrow{\text{CP}_g} e^{i\gamma} \epsilon \phi^*(x') \xrightarrow{U_G} \epsilon \phi^*(x'), \quad (\text{B.9})$$

as we asserted.

We note that our arguments are valid in any basis. Thus, the transformation (54) has the interesting property of being the same, independently of the choice of basis. This holds again up to gauge transformations. We can also see this directly from (41)-(46). We start from (54) and make a basis transformation (41) with  $U \in U(2)$ . Then we get from (44) with  $U_\varphi = \epsilon$

$$U'_\varphi = U \epsilon U^{*-1}. \quad (\text{B.10})$$

We can decompose  $U$  as

$$U = e^{i\gamma/2} \tilde{U} \quad (\text{B.11})$$

with  $\gamma$  real and  $\tilde{U} \in SU(2)$ . For any  $\tilde{U} \in SU(2)$  we have

$$\epsilon^T \tilde{U} \epsilon = \tilde{U}^*. \quad (\text{B.12})$$

Inserting this in (B.10) we get

$$\begin{aligned} U'_\varphi &= e^{i\gamma} \tilde{U} \epsilon \tilde{U}^{*-1} \\ &= e^{i\gamma} \epsilon \epsilon^T \tilde{U} \epsilon \tilde{U}^{*-1} \\ &= e^{i\gamma} \epsilon \tilde{U}^* \tilde{U}^{*-1} \\ &= e^{i\gamma} \epsilon. \end{aligned} \quad (\text{B.13})$$

Again, the factor  $\exp(i\gamma)$  just represents a gauge transformation. With this we have shown directly the basis independence of the  $\text{CP}_g$  transformation of type (i) given in (54).

We go now to a basis where  $E$  is diagonal,

$$E = \text{diag}(\mu_1, \mu_2, \mu_3) \quad (\text{B.14})$$

with the ordering

$$\mu_1 \geq \mu_2 \geq \mu_3. \quad (\text{B.15})$$

For the discussion of the stability of the theory we have to consider the function  $f(u)$  (see (55) of [4]) and the set  $I$  of  $u$  values defined in (70) of [4]. Here we find

$$\begin{aligned} f(u) &= u + \eta_{00}, \\ f'(u) &= 1, \end{aligned} \quad (\text{B.16})$$

$$I = \{0, \mu_1, \mu_2, \mu_3\}. \quad (\text{B.17})$$

Now we go through the criteria spelled out in theorems 1-3 in [4] which tell us when the theory is stable and has the correct EWSB behaviour. In view of theorem 1 of [4] we see that stability in the strong sense requires

$$\begin{aligned} f(0) &= \eta_{00} > 0, \\ f(\mu_a) &= \mu_a + \eta_{00} > 0 \quad (a = 1, 2, 3). \end{aligned} \quad (\text{B.18})$$

If  $\eta_{00} = 0$  or  $\mu_a + \eta_{00} = 0$  for at least one  $a \in \{1, 2, 3\}$  we have to consider the function  $g(u)$ , see (72) of [4]. Here we get

$$g(u) = \xi_0. \quad (\text{B.19})$$

Stability in the *weak sense* requires then  $\xi_0 > 0$ , *marginal* stability  $\xi_0 = 0$ . On the other hand, we have from (117) of [4] the necessary condition for EWSB  $\xi_0 < |\xi|$  which gives here

$$\xi_0 < 0. \quad (\text{B.20})$$

Thus we find that a potential (78) being stable in the *weak sense* or only *marginally* stable cannot have the correct EWSB. In other words: in an acceptable theory of this kind the potential parameters must satisfy (B.18) and (B.20). This already proves the first three relations (80) of theorem 5.

Next we study the stationary points of  $V$ , (78), using the four-dimensional notation (23)-(25). The constraints (22) on the gauge invariant functions read

$$\tilde{\mathbf{K}}(x)^T \tilde{g} \tilde{\mathbf{K}}(x) \geq 0, \quad K_0(x) \geq 0, \quad (\text{B.21})$$

with  $\tilde{g}$  given in (73). For the potential (78) we have, with (B.20) and (B.14),

$$\tilde{\xi} = \begin{pmatrix} \xi_0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \xi_0 < 0, \quad (\text{B.22})$$

$$\tilde{E} = \text{diag}(\eta_{00}, \mu_1, \mu_2, \mu_3). \quad (\text{B.23})$$

The point  $\tilde{\mathbf{K}} = 0$  is always a stationary solution. We now check for the non-trivial stationary points. In the interior of the forward light cone, the stationary points of  $V$  are obtained from (91) of [4],

$$\tilde{E} \tilde{\mathbf{K}} = -\frac{1}{2} \tilde{\xi}, \quad (\text{B.24})$$

$$\tilde{\mathbf{K}}^T \tilde{g} \tilde{\mathbf{K}} > 0, \quad (\text{B.25})$$

$$K_0 > 0. \quad (\text{B.26})$$

From (B.24) we get here

$$\begin{aligned}\eta_{00}K_0 &= -\frac{1}{2}\xi_0, \\ \mu_1K_1 &= 0, \\ \mu_2K_2 &= 0, \\ \mu_3K_3 &= 0.\end{aligned}\tag{B.27}$$

It follows that

$$K_0 = \frac{1}{2\eta_{00}}(-\xi_0) > 0.\tag{B.28}$$

Thus (B.26) is already fulfilled. If

$$\det E = \mu_1\mu_2\mu_3 \neq 0,\tag{B.29}$$

the only stationary point in the interior of the light cone is, therefore,

$$\tilde{\mathbf{K}} = -\frac{\xi_0}{2\eta_{00}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}.\tag{B.30}$$

For  $\det E = 0$  we have regions of stationary points extending from the solution (B.30) to the light cone.

A vacuum with the required EWSB must lie on the forward light cone. We now study all stationary points in this part of the domain, see (96) of [4]:

$$(\tilde{E} - u\tilde{g})\tilde{\mathbf{K}} = -\frac{1}{2}\tilde{\xi},\tag{B.31}$$

$$\tilde{\mathbf{K}}^T \tilde{g}\tilde{\mathbf{K}} = 0,\tag{B.32}$$

$$K_0 > 0.\tag{B.33}$$

From (B.31) we get

$$\begin{aligned}(\eta_{00} - u)K_0 &= -\frac{1}{2}\xi_0, \\ (\mu_1 + u)K_1 &= 0, \\ (\mu_2 + u)K_2 &= 0, \\ (\mu_3 + u)K_3 &= 0.\end{aligned}\tag{B.34}$$

For the functions  $\tilde{f}(u)$  and  $\tilde{f}'(u)$ , (102) and (103) of [4], we find

$$\tilde{f}(u) = -\frac{1}{4} \frac{\xi_0^2}{\eta_{00} - u},\tag{B.35}$$

$$\tilde{f}'(u) = -\frac{1}{4} \frac{\xi_0^2}{(\eta_{00} - u)^2}.\tag{B.36}$$

Now we use theorem 2 of [4] to discuss the stationary points of  $V$ . Since we have here always

$$\tilde{f}'(u) < 0\tag{B.37}$$

there are no solutions of type (IIa). But there are solutions of type (IIb), that is, solutions with

$$\det(\tilde{E} - u\tilde{g}) = 0.\tag{B.38}$$

These occur for

$$u = -\mu_a, \quad a \in \{1, 2, 3\}.\tag{B.39}$$

Indeed, setting  $u = -\mu_3$  we find from (B.34)

$$\begin{aligned}(\eta_{00} + \mu_3)K_0 &= -\frac{1}{2}\xi_0, \\ (\mu_1 - \mu_3)K_1 &= 0, \\ (\mu_2 - \mu_3)K_2 &= 0, \\ 0 \cdot K_3 &= 0.\end{aligned}\tag{B.40}$$

A solution of (B.40) which also satisfies (B.32) and (B.33) is

$$K_0 = K_3 = \frac{-\frac{1}{2}\xi_0}{\eta_{00} + \mu_3}, \quad K_1 = K_2 = 0.\tag{B.41}$$

In fact, any solution of (B.40) which respects (B.32) and (B.33) can be brought to the form (B.41) by a suitable basis change. This holds, in particular, if there are degeneracies of the eigenvalues  $\mu_1, \mu_2$  with  $\mu_3$ .

Of course, we can have solutions of (B.31)-(B.34) analogous to (B.41) for  $u = -\mu_1$  and  $u = -\mu_2$ . For values  $u \notin \{-\mu_1, -\mu_2, -\mu_3\}$  there are, clearly, no solutions of (B.31)-(B.34). Now we remember the ordering of the eigenvalues chosen in (B.15). The solution of (B.31)-(B.34) with the largest Lagrange multiplier  $u_0$  is, therefore, given in (B.41), corresponding to

$$u = u_0 = -\mu_3.\tag{B.42}$$

According to theorem 3 of [4] the theory has the correct EWSB and no zero mass charged Higgses if and only if

$$u_0 = -\mu_3 > 0.\tag{B.43}$$

The vacuum solution is then given by (B.41). We know from the results of [4] that this gives indeed the lowest potential value. Here it is also straightforward to check directly that for instance the stationary point (B.30) in the interior of the light cone gives a higher potential value.

Finally, it is clear that the solution (B.41) violates the  $\text{CP}_g$  symmetry of type (i) spontaneously, since

$$-\mathbf{K} \neq \mathbf{K}.\tag{B.44}$$

With (B.18), (B.20) and (B.43), (B.44) we have completed the investigation of the stability and EWSB behaviour of THDMs with  $\text{CP}_g$  invariance of type (i) and proven theorem 5.

### APPENDIX C: BASIS INDEPENDENT CONDITIONS FOR THE ABSENCE OF SPONTANEOUS $\text{CP}_g$ TYPE (ii) VIOLATION

In this appendix we complete the proof of theorem 6 by showing that the conditions (63)-(66) for the potential parameters together with the conditions (81)-(83) for the

vacuum expectation values are equivalent to the existence of a basis with

$$\xi'_2 = 0, \quad (C.1)$$

$$\eta'_2 = \eta'_{12} = \eta'_{23} = 0, \quad (C.2)$$

$$K'_2 = 0. \quad (C.3)$$

Conditions (C.1)-(C.3) guarantee the existence of a  $CP_g$  type (ii) invariance of both the potential and the vacuum expectation values; see section 4.2.

We note first that (C.1)-(C.3) imply (63)-(66), see appendix A, as well as (81)-(83), as can be seen immediately by direct insertion.

Now we show that from (63)-(66) and (81)-(83) the existence of a basis satisfying (C.1)-(C.3) follows. We show this in two alternative ways. The first proof reveals the number of geometric reflection symmetries for the different cases. The second proof is more formal but also much shorter.

We discuss first the trivial case that the potential parameters satisfy (63)-(66) and the vacuum expectation value is the zero four-vector  $\tilde{\mathbf{K}} = 0$ . Then (81)-(83) are also trivially satisfied. From theorem 3 we see that we can go to a basis where (C.1) and (C.2) hold. Since  $\mathbf{K} = 0$  in our case we have also  $K'_2 = 0$ , q.e.d.

Thus we can turn to the case that  $\tilde{\mathbf{K}} \neq 0$  which implies  $K_0 \neq 0$ ; see (22). Then  $\tilde{\mathbf{K}}$  fulfills the stationarity condition (see (91) and (96) of [4])

$$\tilde{\xi} = -2(\tilde{E} - u\tilde{g})\tilde{\mathbf{K}} \quad (C.4)$$

where  $u$  may be zero. For a theory with the correct EWSB we have  $u = u_0 = m_{H^\pm}^2/(2v_0^2)$ , see (72), but here we keep the discussion general and do not assume this. In components we get from (C.4)

$$\begin{aligned} \xi_0 &= -2(\eta_{00}K_0 - uK_0 + \boldsymbol{\eta}^T \mathbf{K}), \\ \boldsymbol{\xi} &= -2(E\mathbf{K} + u\mathbf{K} + K_0\boldsymbol{\eta}). \end{aligned} \quad (C.5)$$

Consider now a potential with parameters satisfying (63)-(66). We may then choose a basis with  $\boldsymbol{\xi}'$ ,  $\boldsymbol{\eta}'$  and  $E'$  of the form (62) by theorem 3. With a suitable rotation in the 1-3 subspace we can diagonalise  $E'$ . Then we have

$$\boldsymbol{\xi}' = \begin{pmatrix} \xi'_1 \\ 0 \\ \xi'_3 \end{pmatrix}, \quad \boldsymbol{\eta}' = \begin{pmatrix} \eta'_1 \\ 0 \\ \eta'_3 \end{pmatrix}, \quad E' = \text{diag}(\mu_1, \mu_2, \mu_3), \quad (C.6)$$

$$\boldsymbol{\xi}' \times \boldsymbol{\eta}' = \begin{pmatrix} 0 \\ \xi'_3\eta'_1 - \xi'_1\eta'_3 \\ 0 \end{pmatrix}, \quad (C.7)$$

$$\boldsymbol{\xi}' \times E'\boldsymbol{\xi}' = \begin{pmatrix} 0 \\ (\mu_1 - \mu_3)\xi'_1\xi'_3 \\ 0 \end{pmatrix}, \quad (C.8)$$

$$\boldsymbol{\eta}' \times E'\boldsymbol{\eta}' = \begin{pmatrix} 0 \\ (\mu_1 - \mu_3)\eta'_1\eta'_3 \\ 0 \end{pmatrix}. \quad (C.9)$$

In the basis of (C.6) we fulfill already (C.1) and (C.2). It remains to be seen that also (C.3) holds in this basis. Let us first consider the case

$$(a) \quad \boldsymbol{\xi} \times \boldsymbol{\eta} \neq 0 :$$

This implies, of course,  $\boldsymbol{\xi}' \times \boldsymbol{\eta}' \neq 0$ , that is,

$$\xi'_3\eta'_1 - \xi'_1\eta'_3 \neq 0. \quad (C.10)$$

If now (81) holds we get immediately

$$\begin{aligned} (\boldsymbol{\xi}' \times \boldsymbol{\eta}')^T \mathbf{K}' &= 0 \\ \implies (\xi'_3\eta'_1 - \xi'_1\eta'_3)K'_2 &= 0 \\ \implies K'_2 &= 0. \end{aligned} \quad (C.11)$$

Furthermore, we find from (C.8), (C.9) and (C.11) that (82) and (83) are automatically satisfied. We summarise this case. If  $\boldsymbol{\xi} \times \boldsymbol{\eta} \neq 0$  the only possible  $CP_g$  type (ii) symmetry is the reflection on the plane spanned by  $\boldsymbol{\xi}$  and  $\boldsymbol{\eta}$  (see section 3) and this symmetry is respected by the vacuum if and only if (81) holds. In this case (81) implies also (82) and (83). This proves the case (a) of theorem 6.

Next we consider the case

$$(b) \quad \boldsymbol{\xi} \times \boldsymbol{\eta} = 0 :$$

Then (81) is trivially fulfilled. Suppose first that  $\boldsymbol{\xi} \neq 0$ . Then  $\boldsymbol{\eta}$  is proportional to  $\boldsymbol{\xi}$ ,

$$\boldsymbol{\eta} = \lambda\boldsymbol{\xi}. \quad (C.12)$$

For the case of linearly dependent vectors  $\mathbf{K}$  and  $\boldsymbol{\xi}$  we have in particular in the basis defined by (C.6)  $K'_2 = 0$  and (C.3) is proven. So we may assume in the following that  $\mathbf{K}$  and  $\boldsymbol{\xi}$  are linearly independent. Now we distinguish various subcases.

$$(b.1) \quad \boldsymbol{\xi} \times E\boldsymbol{\xi} \neq 0 :$$

The only reflection plane for a symmetry of the potential is spanned by  $\boldsymbol{\xi}$  and  $E\boldsymbol{\xi}$  in this case. We get from (C.8)

$$(\mu_1 - \mu_3)\xi'_1\xi'_3 \neq 0 \quad (C.13)$$

and from (82)

$$(\mu_1 - \mu_3)\xi'_1\xi'_3K'_2 = 0. \quad (C.14)$$

This leads to  $K'_2 = 0$ , q.e.d.

$$(b.2) \quad \boldsymbol{\xi} \times E\boldsymbol{\xi} = 0 :$$

In this case we have

$$(\mu_1 - \mu_3)\xi'_1\xi'_3 = 0. \quad (C.15)$$

Now we distinguish the different cases for the eigenvalues of  $E$ .

(b.2.1)  $\mu_1, \mu_2, \mu_3$  all different:

We get  $\xi'_1 \xi'_3 = 0$ . If, for instance,  $\xi'_1 = 0$  the theory has two reflection symmetries namely in this basis  $R_1$  and  $R_2$  (see (51)). From (C.5) we have

$$\begin{aligned} 0 &= -2(\mu_1 + u)K'_1, \\ 0 &= -2(\mu_2 + u)K'_2. \end{aligned} \quad (\text{C.16})$$

Since we consider here  $\mu_1 \neq \mu_2$  we must have either  $K'_1 = 0$  or  $K'_2 = 0$ . That is, at least one of the reflection symmetries  $R_1$  or  $R_2$  is conserved by the vacuum. In case  $K'_1 = 0$  we can by a change of basis interchange the 1'- and 2'-components and in this way achieve  $K'_2 = 0$ , q.e.d. For  $\xi'_3 = 0$  the argumentation is analogous, involving  $R_1$  and  $R_3$ .

(b.2.2)  $\mu_1 = \mu_2 \neq \mu_3$  :

We get again from (C.15)  $\xi'_1 \xi'_3 = 0$ . For  $\xi'_3 = 0$  the argumentation is as in (b.2.1). For  $\xi'_3 \neq 0$  and  $\xi'_1 = 0$  we may perform a rotation around the 3'-axis such that  $K'_2 = 0$  q.e.d. Note, that  $E'$  is not affected by this rotation since  $\mu_1 = \mu_2$ . In this case we have reflection symmetry on every plane containing the 3'-axis, in particular on the plane spanned by  $\xi'$  and  $\mathbf{K}'$ . The reflection symmetry on this plane clearly is conserved by the vacuum.

(b.2.3)  $\mu_2 = \mu_3 \neq \mu_1$  :

The argumentation is analogous to the case (b.2.2).

(b.2.4)  $\mu_1 = \mu_3 \neq \mu_2$  :

We can, by a rotation around the 2'-axis, leaving  $E'$  diagonal, achieve  $\xi'_1 = \xi'_2 = 0$ ,  $\xi'_3 \neq 0$ . Here  $R_1$  and  $R_2$  are reflection symmetries. Then (C.5) gives

$$\begin{aligned} 0 &= (\mu_1 + u)K'_1, \\ 0 &= (\mu_2 + u)K'_2. \end{aligned} \quad (\text{C.17})$$

Thus, either  $K'_1$  or  $K'_2$  must be zero. In case  $K'_1 = 0$  we can by a change of basis interchange the 1'- and 2'-components and in this way achieve  $K'_2 = 0$ , q.e.d.

(b.2.5)  $\mu_1 = \mu_2 = \mu_3$  :

There is reflection symmetry on all planes containing  $\xi'$ , in particular on the plane spanned by  $\xi'$  and  $\mathbf{K}'$ . This reflection symmetry is obviously unbroken by the vacuum. This proves theorem 6 for the case (b) if  $\xi \neq 0$ . For  $\eta \neq 0$  everything runs analogously using (83) instead of (82).

(b.3)  $\xi = \eta = 0$  :

In this case we have  $\text{CP}_g$  invariance of type (i). There are then at least three  $\text{CP}_g$  type (ii) invariances. We

parameter conditions		number of $\text{CP}_g$ type (ii) reflection symmetries
(a)	$\xi \times \eta \neq 0$	1
(b)	$\xi \times \eta = 0$	
(b.1)	$\xi \neq 0, \xi \times E\xi \neq 0$ $\eta \neq 0, \eta \times E\eta \neq 0$	1 1
(b.2)	$\xi \neq 0, \xi \times E\xi = 0$ or $\eta \neq 0, \eta \times E\eta = 0$ , eigenvalues of E: $\mu_1, \mu_2, \mu_3$	
(b.2.1)	$\mu_1, \mu_2, \mu_3$ all different	2
(b.2.2)	$\mu_1 = \mu_2 \neq \mu_3$	2 or $\infty$
(b.2.3)	$\mu_2 = \mu_3 \neq \mu_1$	2 or $\infty$
(b.2.4)	$\mu_1 = \mu_3 \neq \mu_2$	2
(b.2.5)	$\mu_1 = \mu_2 = \mu_3$	$\infty$
(b.3)	$\xi = 0, \eta = 0$ , $\mu_1, \mu_2, \mu_3$ : all different at least 2 equal	3 $\infty$

TABLE I: The  $\text{CP}_g$  type (ii) transformations are described by reflections on planes. The table lists the number of these symmetries for a potential satisfying (63)-(66) depending on the different cases for the parameters. The vacuum is invariant under at least one of the symmetries if and only if (81)-(83) hold. The numbering of the eigenvalues  $\mu_1, \mu_2, \mu_3$  of  $E$  is chosen such that  $\mu_2 = \eta'_{22}$  in a basis where  $\xi', \eta'$  and  $E'$  have the form (62).

have here from (C.5)

$$\begin{aligned} 0 &= (\mu_1 + u)K'_1, \\ 0 &= (\mu_2 + u)K'_2, \\ 0 &= (\mu_3 + u)K'_3. \end{aligned} \quad (\text{C.18})$$

If not all  $\mu_a$  are equal this implies that at least one  $K'_a = 0$  ( $a \in \{1, 2, 3\}$ ). By a change of basis we can always achieve that  $K'_2 = 0$ , q.e.d. If  $\mu_1 = \mu_2 = \mu_3$  we have reflection symmetry of the potential on any plane. The reflection symmetries on all planes containing  $\mathbf{K}'$  are respected by the vacuum. This completes the first proof of theorem 6.

From the detailed discussion above we also found the number of independent reflection symmetries, that is, type (ii)  $\text{CP}_g$  transformations, which occur for the various cases. This is summarised in table I where it is always supposed that the potential parameters satisfy (63)-(66).

Now we present an alternative and more formal proof that from (63)-(66) and (81)-(83) the existence of a basis satisfying (C.1)-(C.3) follows. For the stationary point  $\bar{\mathbf{K}} = 0$ , which leaves the electroweak symmetry unbroken, the proof is trivial. We shall now prove the statement



for all other stationary points, in particular for solutions with the required EWSB. We will use the fact that any stationary point  $\tilde{\mathbf{K}} \neq 0$  fulfills a stationarity condition of the form (C.5) with a specific value of  $u$ . As a preparation we first show that certain additional invariants vanish. Replacing  $\xi$  in (81) via the stationarity condition (C.5) we find

$$(\eta \times (E\mathbf{K}))^T \mathbf{K} = 0. \quad (\text{C.19})$$

This implies

$$(\xi \times (E\mathbf{K}))^T \mathbf{K} = 0, \quad (\text{C.20})$$

which can be seen by replacing  $\xi$  via (C.5). Next we show that

$$(\eta \times (E\xi))^T \mathbf{K} = 0. \quad (\text{C.21})$$

If  $\eta$  and  $\mathbf{K}$  are linearly dependent, (C.21) follows immediately. In the other case we replace  $\xi$  in (C.21) by a linear combination of  $\eta$  and  $\mathbf{K}$ , which is possible by (81). Using (83) and (C.19), (C.21) follows. Similarly we find

$$(\xi \times (E\eta))^T \mathbf{K} = 0, \quad (\text{C.22})$$

using (81), (82) and (C.20). The relation

$$(E\mathbf{K} \times (E\xi))^T \mathbf{K} = 0 \quad (\text{C.23})$$

follows after substitution of  $E\mathbf{K}$  via (C.5) from (82) and (C.21). Similarly we find

$$(E\mathbf{K} \times (E\eta))^T \mathbf{K} = 0 \quad (\text{C.24})$$

using (C.5), (83) and (C.22). We find

$$(\mathbf{K} \times (E\mathbf{K}))^T E^2 \mathbf{K} = 0 \quad (\text{C.25})$$

by replacing  $E\mathbf{K}$  in the term  $E^2 \mathbf{K}$  via (C.5) since (C.23) and (C.24) hold.

In the case that  $\xi$  and  $\eta$  are linearly independent, we may choose a basis of the form (62) by theorem 3. From (81) follows immediately that we have  $K_2 = 0$  in this basis.

In the case that  $\xi$  is a multiple of  $\eta$  we note that (83), (C.19), (C.25) and (66),

$$\begin{aligned} (\mathbf{K} \times \eta)^T E\mathbf{K} &= 0, & (\mathbf{K} \times (E\mathbf{K}))^T E^2 \mathbf{K} &= 0, \\ (\mathbf{K} \times \eta)^T E\eta &= 0, & (\eta \times (E\eta))^T E^2 \eta &= 0, \end{aligned} \quad (\text{C.26})$$

are equal to the explicit CP conservation conditions (63)-(66) if we replace  $\xi$  by  $\mathbf{K}$  in the latter. Using the proof of theorem 3 we find that there is a basis with  $\eta'_2 = K'_2 = \eta'_{12} = \eta'_{23} = 0$  and thus also  $\xi'_2 = 0$ .

In the case that  $\eta$  is a multiple of  $\xi$  we use (82), (C.20), (C.25) and (65),

$$\begin{aligned} (\mathbf{K} \times \xi)^T E\mathbf{K} &= 0, & (\mathbf{K} \times (E\mathbf{K}))^T E^2 \mathbf{K} &= 0, \\ (\mathbf{K} \times \xi)^T E\xi &= 0, & (\xi \times (E\xi))^T E^2 \xi &= 0. \end{aligned} \quad (\text{C.27})$$

Replacing  $\eta$  by  $\mathbf{K}$  everywhere in the proof of theorem 3 we see that we can find a basis with  $\xi'_2 = K'_2 = \eta'_{12} = \eta'_{23} = 0$  and thus also  $\eta'_2 = 0$ . This completes the second proof of theorem 6.

We compared our conditions (81)-(83) for absence of spontaneous CP violation with those of theorem 4 in [14]. The triple product in (81) equals  $-(v/2)^4 \text{Im } J_1$  in their notation, the other invariants in [14] and our conditions have no one-to-one correspondence. However, we find complete agreement between our conditions for absence of spontaneous CP violation and those of [14] taking into account the respective full set of equations, that is, including the explicit CP-conservation conditions and the stationarity equations. This equivalence may be obtained via *Groebner basis* computations. Note however the comment in section 4.2 after theorem 6 that ‘‘absence of spontaneous CP violation’’ is not quite an appropriate formulation. From the discussion of the case (b) above and from table I we see that, indeed, a theory can have more than one  $\text{CP}_g$  type (ii) invariance. One of these symmetries is always respected by the vacuum if (81)-(83) hold, but at the same time others may be broken spontaneously. We also compared our conditions (81)-(83) to the corresponding conditions a)-c) in [15] and find agreement up to (83), which is not contained in the latter set of criteria. The condition c) of [15] is no further restriction since it is automatically fulfilled by the stationarity condition; see (C.20). Further, we do find examples where omitting (83) matters, that is examples satisfying the conditions of [15] but having spontaneous breaking of all CP symmetries of the potential.

Let us now come back to Tab. I and the cases of multiple  $\text{CP}_g$  symmetries of type (ii). Suppose we have in a theory two invariances of this type denoted by  $\text{CP}_g^{(ii)}$  and  $\overline{\text{CP}}_g^{(ii)}$ . Then the product  $S \equiv \overline{\text{CP}}_g^{(ii)} \circ \text{CP}_g^{(ii)}$  is a conventional Higgs flavour symmetry. Indeed, from the field transformation (42) we get

$$\begin{aligned} \phi(x) &\xrightarrow{\text{CP}_g^{(ii)}} U_\varphi \phi^*(x') \\ \phi(x) &\xrightarrow{\overline{\text{CP}}_g^{(ii)}} U'_\varphi \phi^*(x') \end{aligned} \quad (\text{C.28})$$

and

$$\phi(x) \xrightarrow{S} U'' \phi(x) \quad \text{with } U'' = U'_\varphi U_\varphi^*. \quad (\text{C.29})$$

Here  $U_\varphi$ ,  $U'_\varphi$  and  $U''$  are all elements of  $U(2)$ . Thus we see that in the cases of 2,3 or an infinite number of  $\text{CP}_g$  transformations of type (ii) as listed in Tab. I there is a corresponding number of Higgs flavour symmetries. The possibility of a discrete ambiguity in the definition of a generalised CP transformation as a symmetry of the theory was also noted in [14].

Finally we discuss further the relation of the  $\text{CP}_g$  symmetries of type (i) and (ii). Let us consider the generic case of a theory where the Lagrangian is invariant under the type (i) transformation, that is the case (b.3) from Tab. I with  $\mu_1, \mu_2, \mu_3$  all different. As we have shown

in appendix B, the  $\text{CP}_g$  transformation of type (i) of the fields is given in any basis by (54). Clearly, we can consider this as product of the standard  $\text{CP}_s$  transformation (27) and the Higgs flavour transformation induced by  $\epsilon$

$$\begin{aligned}\varphi_1(x) &\rightarrow \varphi_2(x), \\ \varphi_2(x) &\rightarrow -\varphi_1(x).\end{aligned}\tag{C.30}$$

But note that in a given basis *neither* this  $\text{CP}_s$  *nor* the transformation (C.30) will in general be symmetries of the theory. On the other hand we see from Tab. I that a theory with  $\text{CP}_g$  invariance of type (i) automatically has three  $\text{CP}_g$  invariances of type (ii). The latter are the reflections on the coordinate planes in  $\mathbf{K}$  space only in the special basis where  $E$  is diagonal. There are also three corresponding discrete Higgs flavour symmetries of the type of a product of the  $\text{CP}_g$  symmetry of type (i) and one of type (ii). But this should be considered as a finding a posteriori which is valid for the Higgs sector of the theory taken in isolation. In the companion paper [23] we find that for the complete theory, that is, the theory including fermions, the  $\text{CP}_g$  symmetry of type (i) does in general not automatically imply invariance under the above mentioned  $\text{CP}_g$  transformations of type (ii). Thus, both from a conceptual point of view and from exploring physical consequences, the  $\text{CP}_g$  transformations of type (i) and (ii) should be considered independently for their own sake.

#### APPENDIX D: THEORIES WITH $\text{CP}_g$ TYPE (ii) INVARIANCE

Here we study the stability and EWSB behaviour of models having a  $\text{CP}_g$  symmetry of type (ii). According to the discussion in section 3.2 we can then go to a basis (62) where  $E'$  is already partly diagonalised. By a change of basis in the 1'-3' plane we can diagonalise  $E'$  completely without changing the  $\text{CP}_g$  transformation which is  $R_2$  (32) in this basis. We then have

$$E' = \text{diag}(\mu_1, \mu_2, \mu_3), \tag{D.1}$$

with  $\eta'_{22} = \mu_2$  unchanged by the rotation in the 1'-3' plane. In the following all formulae refer to this basis where we drop the prime for ease of notation. Then we get for the four-vector  $\tilde{\xi}$  and the  $4 \times 4$  matrix  $\tilde{E}$  defined in (25)

$$\tilde{\xi} = \begin{pmatrix} \xi_0 \\ \xi_1 \\ 0 \\ \xi_3 \end{pmatrix}, \tag{D.2}$$

$$\tilde{E} = \begin{pmatrix} \eta_{00} & \eta_1 & 0 & \eta_3 \\ \eta_1 & \mu_1 & 0 & 0 \\ 0 & 0 & \mu_2 & 0 \\ \eta_3 & 0 & 0 & \mu_3 \end{pmatrix} \tag{D.3}$$

with the potential given by (24). We must check the stability of the potential. Suppose this has been done, for instance by using theorem 1 of [4].

For a theory to have the correct EWSB and no zero mass charged Higgs fields the global minimum of  $V$  must be a solution of (B.31)-(B.33), that is  $\tilde{\mathbf{K}}$  must be a light-like four-vector. The corresponding Lagrange multiplier  $u_0$  must be positive

$$u_0 > 0, \tag{D.4}$$

and it must be the largest Lagrange multiplier of all solutions of (B.31)-(B.33). According to theorem 3 of [4] these conditions are indeed not only necessary but also sufficient for the determination of the global minimum of an acceptable theory.

Now we can write out (B.31) in components. For  $K_2$  we find

$$(\mu_2 + u)K_2 = 0. \tag{D.5}$$

Spontaneous violation of the  $\text{CP}_g$  type (ii) symmetry corresponding to  $R_2$  in this basis means  $K_2 \neq 0$ . Clearly, a solution of (D.5) with  $K_2 \neq 0$  requires

$$u = -\mu_2. \tag{D.6}$$

This can correspond to the true vacuum solution only if  $u = u_0 > 0$ . Thus, we find as necessary condition for spontaneous violation of this  $\text{CP}_g$  type (ii) symmetry from (D.4) and (D.5) that the eigenvalue  $\mu_2 = \eta_{22}$  of  $E$  must be negative,

$$\mu_2 = \eta_{22} < 0. \tag{D.7}$$

To prove that this  $\text{CP}_g$  symmetry is spontaneously broken one still has to check if, indeed, (B.31)-(B.33) have a solution for  $u = -\mu_2$  and whether this is the solution with the largest Lagrange multiplier  $u = u_0$ . The above results are summarised in theorem 7 in section 4.2.

Let us finally consider a potential with parameters as in (D.2), (D.3) having (at least) two stationary solutions on the light cone; see (B.31)-(B.33). We suppose that the  $\text{CP}_g$  symmetry corresponding to the reflection  $R_2$  in this basis is respected by one solution  $\tilde{K}^{\text{CP}}$  with  $K_2^{\text{CP}} = 0$  and violated by the other solution  $\tilde{K}^{\text{CP}}$  through  $K_2^{\text{CP}} \neq 0$ . We denote the corresponding Lagrange multipliers by  $u_{\text{CP}}$  and  $u_{\text{CP}} = -\mu_2$ . Perturbing the  $\text{CP}_g$  conserving point by a small amount ( $0 < \varepsilon \ll 1$ ) within the light cone according to

$$\tilde{K}^{\text{CP}} \rightarrow \tilde{K}^{\text{CP}} + K_0^{\text{CP}} \begin{pmatrix} \sqrt{1 + \varepsilon^2} - 1 \\ 0 \\ \pm \varepsilon \\ 0 \end{pmatrix}, \tag{D.8}$$

we find for the potential value

$$V(\tilde{K}^{\text{CP}}) \rightarrow V(\tilde{K}^{\text{CP}}) + (u_{\text{CP}} + \mu_2) (K_0^{\text{CP}})^2 \varepsilon^2 + \mathcal{O}(\varepsilon^4) \tag{D.9}$$

after employing the corresponding stationarity condition (B.31) with  $u = u_{\text{CP}}$ . Therefore, the  $\text{CP}_g$  conserving point can only be a (local) minimum if  $u_{\text{CP}} + \mu_2 \geq 0$ , that is, if  $u_{\text{CP}} \geq u_{\text{CP}^*}$ . From (123) in [4] we know that a higher Lagrange multiplier means a lower potential value. To summarise, if the potential has a  $\text{CP}_g$  conserving (local) minimum, there can be no stationary points with lower values of the potential which violate this symme-

try. This result was found before, see [29] and references therein. While the existence of a  $\text{CP}_g$  conserving light-like minimum implies that the global minimum has these properties too, there are cases with more than one  $\text{CP}_g$  conserving light-like minimum; see Fig. 3 of [4]. Therefore, a determination of the actual global minimum is still necessary in general.

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